

Open Quantum Dynamics: Complete Positivity and Entanglement

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We review the standard treatment of open quantum systems in relation to quantum entanglement, analyzing, in particular, the behaviour of bipartite systems immersed in a same environment. We first focus upon the notion of complete positivity, a physically motivated algebraic constraint on the quantum dynamics, in relation to quantum entanglement, *i.e.* the existence of statistical correlations which can not be accounted for by classical probability. We then study the entanglement power of heat baths versus their decohering properties, a topic of increasing importance in the framework of the fast developing fields of quantum information, communication and computation. The presentation is self contained and, through several examples, it offers a detailed survey of the physics and of the most relevant and used techniques relative to both quantum open system dynamics and quantum entanglement.

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1. Introduction

Standard quantum mechanics mainly deals with *closed* physical systems that can be considered isolated from any external environment, the latter being generically a larger system consisting of (infinitely) many degrees of freedom. The time-evolution of closed systems is described by one-parameter groups of unitary operators embodying the reversible character of the dynamics. On the contrary, when a system S interacts with an environment E in a non-negligible way, it must be treated as an *open quantum system*, namely as a subsystem embedded within E , exchanging with it energy and entropy, and whose time-evolution is irreversible.^a

In general, the time-evolution of S is inextricably linked to that of E . The compound system $S + E$ is closed and develops reversibly in time; however, the global time-evolution rarely permits the extraction of a meaningful dynamics for the

^aThe literature on the theory of open quantum systems and their phenomenological applications is vast; in the References, only papers that are strictly relevant to the present exposition are therefore included. We start by providing a list of general reviews and monographs on the topic, Refs.[1-16], where additional references can be found.

system S alone. This can be done if the coupling among subsystem and environment is sufficiently weak, in which case physically plausible approximations lead to *reduced dynamics* that involve only the S degrees of freedom and are generated by *master equations*. Such reduced dynamics provide effective descriptions of how E affects the time-evolution of S which, on time-scales that are specific of the given physical contexts, typically incorporates dissipative and noisy effects.

In order to better appreciate the physical motivations underlying the concept of reduced dynamics, classical Brownian motion is a helpful guide.¹⁷ On the fast microscopic time-scale, the scattering of the environment particles off the mesoscopic Brownian particle S are described by a reversible dynamics. On the slower mesoscopic time-scale, the memory effects related to microscopic interactions are averaged out and the effective dynamics of S is diffusion, that is an irreversible Markov process. Physically speaking, on the slow time-scale the environment degrees of freedom act as a sink where S dissipates energy, but also as a source of (white) noise with long-run stabilizing effects. We shall see that, under certain conditions, irreversible Markovian time-evolutions, leading to dissipation and noise, find a concrete description in quantum mechanics by means of the so-called *quantum dynamical semigroups*.

Classical Brownian motion indicates that, when the typical time-scale of S is much larger than the time-scale governing the decay of time-correlations of the environment, then E can be described as an effective source of damping and noise. In the framework of open quantum systems, this possibility is technically implemented either by letting the typical variation time of S , τ_S , go to infinity, while the environment correlation time τ_E stays finite, or by letting τ_E go to zero, while τ_S stays finite.³ As we shall see, these two regimes give rise to two different procedures to arrive at a reduced dynamics described by Markovian semigroups: the so-called *weak coupling* and *singular coupling* limits.

Since their first appearance, open quantum systems have been providing models of non-equilibrium quantum systems in diverse fields as chemical-physics, quantum optics and magnetic resonance. Recently, the rapid development of the theory of quantum information, communication and computation^b has revived the interest in open quantum systems in relations to their decohering properties, but also in their capacity of creating entanglement in multi-partite systems immersed in certain environments. The typical open quantum systems in these contexts are n -level systems, like atoms, photons or neutrons embedded in optical cavities or heat baths consisting of bosonic or fermionic degrees of freedom. These will be the cases studied in this review.

It is worth mentioning that, more in general, one can expect dissipative and noisy effects to affect also the behaviour of elementary particle systems, like neutral mesons, neutrinos and photons: the ensuing irreversibility is the emerging result of the dynamics of fundamental degrees of freedom at very short distances, typically

^bFor general reviews on these topics, see Refs.[18-20].

the Planck-scale.²¹ These effects produce distinctive signatures in the behaviour of selected physical observables, allowing direct experimental testing (for specific treatments and further details, see Refs.[22-32]).

Providing different concrete experimental contexts to study dissipative quantum dynamics is important not only from the point of view of the physics of open quantum systems, but also for the investigations of certain still debated aspects of these generalized time-evolutions, specifically regarding the property of positivity *v.s.* that of complete positivity, notions on which we now briefly elaborate.

A primary consequence of a noisy environment E is that pure states of S , that is projections onto Hilbert space vectors, are usually mapped into mixtures of projections, that is into generic density matrices. These are operators with discrete spectrum consisting of positive eigenvalues summing up to one; within the statistical interpretation of quantum mechanics, they represent probabilities and are used to calculate the mean values of all physical observables pertaining to S . In order to be physically consistent, any reduced dynamics must thus correspond to maps on the space of states of S that preserve for all times the positivity of the spectrum. In other words, any physically consistent reduced dynamics must transform density matrices into density matrices at all (positive) times.

The simplest way to arrive at dissipative time-evolutions is to construct them as solutions of suitable master equations of *Liouville* type: $\partial_t \rho_t = \mathbb{L}[\rho_t]$, where \mathbb{L} operates linearly on the density matrices ρ_t describing the state of S at time t . These are usually obtained by first tracing away the environment degrees of freedom, an operation that leads to a dynamical equation plagued in general by non-linearities, secular terms and memory effects. Non-linearities and secular terms can be eliminated by requiring the initial states of S to be statistically decoupled from an initial reference state of E . On the other hand, memory effects are expected to be relevant on short time-scales and to become negligible if one looks at phenomena associated to longer time-scales when those effects have already died out.

In technical terms, studying the time-evolution on a slow time-scale, thus neglecting memory effects, means operating a so-called *Markovian approximation*; this gives an efficient description of the reduced dynamics of S in terms of time-evolutions consisting of one-parameter semigroups of linear maps $\gamma_t = \exp(t\mathbb{L})$, $t \geq 0$. These are maps that, acting on all possible initial density matrices ρ , provide their time-evolved partners $\rho_t \equiv \gamma_t[\rho]$ at time t . The dynamical maps γ_t are formally obtained by exponentiating the *generators* \mathbb{L} , so that $\gamma_{t+s} = \gamma_t \circ \gamma_s = \gamma_s \circ \gamma_t$, $s, t \geq 0$.

In most open systems, the memory effects are due to a transient regime with a very small time-span that makes Markov approximations legitimate; nevertheless, if not carefully performed, a likely outcome is a physically inconsistent time-evolution that does not preserve the positivity of the spectrum of all initial density matrices. As we shall explicitly see in the following, brute force Markov approximations may provide semigroups of linear maps γ_t that at some time transform an initial state ρ into an operator ρ_t with negative eigenvalues, which can not be used as probabilities.

In other words, without due care in the derivation, one is very likely to obtain γ_t that do not transform the space of states into itself. In order to avoid the appearance of negative probabilities, one has to perform Markov approximations that lead to semigroups of linear maps that preserve positivity: maps with such a property are called *positive*.

Remarkably enough, both the mathematical property of linear maps of being positive and the derivation of positive dynamical maps through Markov approximations are elusive and still not fully understood. However, positivity is not the end of the story and even a semigroup of positive linear maps would not be fully physical consistent. Indeed, suppose S is coupled to an inert system A , a so-called *ancilla*, with which it does not interact; then, the time-evolution of the compound system $S + A$ is $\gamma_t \otimes \text{id}_A$. The identity map id_A means that the coupling to the ancilla does not possess a dynamical character: it manifests itself purely in terms of statistical correlations, *i.e.* in the possibility of initial correlations between S and A .

It turns out that the positivity of γ_t does not guarantee the positivity of $\gamma_t \otimes \text{id}_A$; namely, even if γ_t transforms any initial state of S into a state, $\gamma_t \otimes \text{id}_A$ can map an initial state of $S + A$ into an operator which exhibits negative eigenvalues and can not thus be interpreted as a physical state of $S + A$. In order to be sure that, for whatever ancilla A , the evolution $\gamma_t \otimes \text{id}_A$ consistently maps any state of $S + A$ into a state, γ_t must be a so-called *completely positive* map for all $t \geq 0$, a stronger property than positivity.

We shall show that the ultimate physical meaning of complete positivity lies in its relation to the existence of *entangled states*, the foremost instance of them being a vector state with a singlet-like structure that can not be written as a tensor product of vector states. Indeed, the only states that could be mapped out of the state-space by $\gamma_t \otimes \text{id}_A$ and thus made not anymore acceptable as physical states, are only the entangled states of $S + A$.

Unitary time-evolutions are automatically completely positive, while this is not in general true of many Markovian approximations encountered in the literature on open quantum systems. Complete positivity or its absence depend on the way Markovian approximations are performed. Since the coupling of the open system S with a generic ancilla can not be excluded, the request of complete positivity is hardly dismissible when one deals with dynamical semigroups. Such a request has strong mathematical and physical consequences in that the structure of the generator \mathbb{L} is fixed; from this a typical hierarchy among the characteristic relaxation times of S follows. The uncontrollability of the ancilla and the abstractness of the whole justification of why complete positivity should be physically compelling is scarcely appealing from a concrete point of view, all the more so since complete positivity strongly constrains the reduced dynamics.

However, we shall see that the same physical inconsistencies typical of the abstract contexts, $S + A$, also occur when one considers not a generic inert ancilla A , but another system S also immersed in E , that is an open quantum system $S + S$. If the two parties weakly interact with E and do not interact between themselves,

the dissipative time-evolution of the compound system $S + S$ is of the form $\gamma_t \otimes \gamma_t$ instead of the abstract $\gamma_t \otimes \text{id}_A$ and the setting becomes more physical.

Consider, for instance, two optically active non-interacting atoms (or molecules) initially prepared in an entangled polarization state and evolving in contact with a same heat bath, weakly coupled to them. Then, if the dynamical maps γ_t describing the dissipative evolution of each single atom is not completely positive, there are physically admissible initial entangled states of the two atoms that, after some time, lose their interpretation as physical states because of the emergence of negative probabilities generated by $\gamma_t \otimes \gamma_t$.

The rising of quantum entanglement as a physical resource enabling the performance of quantum information and computation tasks otherwise impossible as teleportation, superdense coding, quantum cryptography and quantum computation, has spurred the investigation of how entanglement can be generated, detected and manipulated. Contrary to standard expectations, the presence of an environment, and thus of noise, need not necessarily spoil the entanglement properties of states of systems immersed in it, but in some cases can even have entangling effects. Using the previous examples, the two optically active atoms could be prepared in an initial separable state without either classical or quantum correlations and put into a heat bath. The covariance structure of the bath correlation functions may be such that not only the two atoms become entangled, but also such that a certain amount of entanglement survives over longer and longer times. The reason is not hard to see: even if not directly coupled, two systems immersed in a same heat bath can interact through the bath itself; it does then depend on how strong this indirect interaction is with respect to the decoherence whether entanglement can be created and maintained.

The plan of this review is as follows. In Section 2, we shall set the mathematical framework appropriate to the description of open quantum systems and to the derivation of their reduced dynamics, with particular emphasis on the notions of positive and completely positive maps on the space of states.

In Section 3, we shall review standard derivations of dissipative semigroups, discussing the role of the Markov approximations in achieving completely positive dynamical maps or not and illustrating the physical inconsistencies arising from lack of complete positivity.

In Section 4, we shall address the entangling effects that the presence of an environment may have on non-directly interacting bipartite systems. All topics will be illustrated by means of concrete examples.

2. Open Quantum Systems: Mathematical Setting

In the first part of this Section we review some basic kinematics and dynamics of open quantum systems, fixing, in passing, the necessary notation. In the second part we shall discuss positivity and complete positivity of linear maps with particular emphasis on their relations with quantum entanglement.

We shall consider finite (n -level) open quantum systems S ; they are described by means of n -dimensional Hilbert spaces \mathbb{C}^n , where \mathbb{C} is the set of complex numbers, and by the algebras $M_n(\mathbb{C})$ of $n \times n$ complex matrices X .^c

The hermitian matrices $X = X^\dagger$ correspond to the system observables and their mean values depend on the physical states of S . The latter can be divided into two classes, the *pure states* described by projectors $P_\psi = |\psi\rangle\langle\psi|$ onto normalized vectors $|\psi\rangle \in \mathbb{C}^n$ and the *statistical mixtures* described by *density matrices*, i.e. by linear convex combinations of (not necessarily orthogonal) projectors

$$\rho = \sum_j \lambda_j P_{\psi_j}, \quad \lambda_j \geq 0, \quad \sum_j \lambda_j = 1. \quad (1)$$

In the following we shall refer to them simply as states, specifying whether they are pure or mixtures when necessary; further,

$$\text{Tr}(\rho) = \sum_j \lambda_j = 1, \quad (2)$$

where Tr represents the trace-operation $\text{Tr}(X) = \sum_i \langle i|X|i\rangle$, with $|i\rangle, i = 1, 2, \dots, n$ any orthonormal basis in \mathbb{C}^n .

Projectors and density matrices are thus normalized hermitian elements of $M_n(\mathbb{C})$; further, they are positive semi-definite matrices.

Definition 2.1 *A matrix $X^\dagger = X \in M_n(\mathbb{C})$ is positive semi-definite if*

$$\langle\psi|X|\psi\rangle \geq 0, \quad \forall \psi \in \mathbb{C}^n. \quad (3)$$

Positive semi-definite matrices will be called positive for sake of simplicity and denoted by $X \geq 0$; their spectrum necessarily consists of positive (non-negative) eigenvalues.

Quantum states are thus positive, normalized operators; the eigenvalues of the pure ones P_ψ are 1 (non-degenerate) and 0 ($n-1$ times degenerate), while those of density matrices are generic $0 \leq r_j \leq 1, j = 1, 2, \dots, n$, such that $\sum_j r_j = 1$. It follows that pure states and mixtures are distinguished by the fact that $\rho^2 = \rho$ if and only if $\rho = P_\psi$ for some $|\psi\rangle \in \mathbb{C}^n$. Also, the eigenvalues of a density matrix ρ correspond to the weights λ_j in (1) if and only if (1) is the spectral representation of ρ , the $|\psi_j\rangle$ are its eigenstates and the P_{ψ_j} the corresponding orthogonal eigenprojectors, $P_{\psi_j}P_{\psi_k} = \delta_{jk}P_{\psi_j}$.

Given a state ρ , the mean value $\langle X \rangle_\rho$ of any observable $X = X^\dagger \in M_n(\mathbb{C})$ is calculated as follows:

$$\langle X \rangle_\rho \equiv \text{Tr}(\rho X) = \sum_j \lambda_j \langle\psi_j|X|\psi_j\rangle. \quad (4)$$

The previous considerations constitute the bulk of the statistical interpretation of quantum mechanics:

^cGeneral monographs on quantum physics relevant for our exposition are Refs.[33,36,37].

Given the spectral decomposition of a state,

$$\rho = \sum_{i=1}^n r_i |r_i\rangle\langle r_i|, \quad \sum_{i=1}^n r_i = 1, \quad \langle r_i | r_j \rangle = \delta_{ij}, \quad (5)$$

the eigenvalues r_i constitute a probability distribution which completely defines the statistical properties of the system.

Accordingly, one associates to quantum states the von Neumann entropy,

$$S(\rho) = -\text{Tr}(\rho \log \rho) = -\sum_{i=1}^n r_i \log r_i, \quad (6)$$

which measures the amount of uncertainty about the actual state of S . It turns out that $S(\rho) = 0$ if and only if $\rho^2 = \rho$, otherwise $0 < S(\rho) \leq \log n$.

Remark 2.1 Density matrices form a convex subset $\mathcal{S}(S) \subset M_n(\mathbb{C})$ which we shall refer to as the state-space of S . Namely, combining different mixtures $\sigma_j \in \mathcal{S}(S)$ with weights $\lambda_j \geq 0$, $\sum_j \lambda_j = 1$, into the convex combination $\sum_j \lambda_j \sigma_j$, the latter also belongs to $\mathcal{S}(S)$. Pure states are extremal elements of $\mathcal{S}(S)$, that is they can not be convexly decomposed, while with them, by linear convex combinations, one generates the whole of the state-space. \square

2.1. Reversible and Irreversible Dynamics

The state-space and the algebra of observables fix the kinematics of S . Its dynamics as a closed system is determined by a Hamiltonian operator $H \in M_n(\mathbb{C})$ through the Schrödinger equation (we shall set $\hbar = 1$):

$$\partial_t |\psi_t\rangle = -i H |\psi_t\rangle. \quad (7)$$

By direct inspection, first on projectors P_ψ and then on mixtures, this gives rise to the so-called Liouville-von Neumann equation on the state-space $\mathcal{S}(S)$:

$$\partial_t \rho_t = -i [H, \rho_t], \quad (8)$$

whose solution, with initial condition $\rho_{t=0} = \rho$, is

$$\rho_t = U_t \rho U_{-t}, \quad U_t = e^{-iHt}. \quad (9)$$

Denoting by $\rho \mapsto \mathbb{U}_t[\rho] \equiv \rho_t$ the dynamical map (9) and by

$$\rho \mapsto \mathbb{L}_H[\rho] \equiv -i [H, \rho], \quad (10)$$

the linear action of the generator on the left hand side of (8), the Schrödinger unitary dynamics amounts to exponentiation of \mathbb{L} :

$$\rho_t = \mathbb{U}_t[X] = e^{t\mathbb{L}_H}[\rho] = \sum_k \frac{t^k}{k!} \underbrace{\mathbb{L}_H \circ \mathbb{L}_H \cdots \circ \mathbb{L}_H}_{\mathbb{L}_H^k}[\rho], \quad (11)$$

where \circ means compositions of maps. Therefore, the dynamical maps \mathbb{U}_t form a one-parameter group of linear maps on $\mathcal{S}(S)$: $\mathbb{U}_t \circ \mathbb{U}_s = \mathbb{U}_{t+s}$ for all $t, s \in \mathbb{R}$. This fact mathematically describes the reversible character of the unitary Schrödinger dynamics; in particular, the dynamical maps \mathbb{U}_t can be inverted, preserve the spectrum of all states ρ , leave the von Neumann entropy invariant and transform pure states into pure states:

$$\rho^2 = \rho \implies (\mathbb{U}_t[\rho])^2 = \mathbb{U}_t[\rho] . \quad (12)$$

Remark 2.2 One can pass from the Schrödinger to the Heisenberg time-evolution through the definition of mean values (4) and the so-called *duality relation*

$$\mathrm{Tr}[\mathbb{U}_t[\rho] X] = \mathrm{Tr}[\rho \mathbb{U}_t^*[X]] , \quad (13)$$

which holds for all $\rho \in \mathcal{S}(S)$, $X \in M_n(\mathbb{C})$ and defines the *dual linear map* \mathbb{U}_t^* . The latter acts on $M_n(\mathbb{C})$ as

$$X \mapsto \mathbb{U}_t^*[X] = U_{-t} X U_t = e^{-t\mathbb{L}_H}[X] . \quad (14)$$

□

The unitary dynamics is not the only dynamical transformation affecting quantum states. According to the postulates of quantum mechanics, if the state of S is $|\psi\rangle\langle\psi|$, upon measuring the (spectralized) observable $X = \sum_{i=1}^n x_i |x_i\rangle\langle x_i|$, then

- the eigenvalues x_i are obtained with probabilities $|\langle x_i | \psi \rangle|^2$,
- if the measure gives x_i , then the post-measurement state of S is $|x_i\rangle\langle x_i|$.

It follows that, by repeating the measurement many times on copies of S equally prepared in the pure state $|\psi\rangle\langle\psi|$ and collecting all the resulting post-measurement states, the outcome is a physical mixture described by the density matrix

$$\sum_{i=1}^n |\langle x_i | \psi \rangle|^2 |x_i\rangle\langle x_i| = \sum_{i=1}^n |x_i\rangle\langle x_i| \left(|\psi\rangle\langle\psi| \right) |x_i\rangle\langle x_i| . \quad (15)$$

Setting $P_i = |x_i\rangle\langle x_i|$ and extending (15) linearly to any density matrix $\rho \in \mathcal{S}(S)$, one gets the following linear map on $\mathcal{S}(S)$:

$$\rho \mapsto \mathbb{P}[\rho] = \sum_{i=1}^n P_i \rho P_i . \quad (16)$$

This map is a mathematical description of the so-called *wave-packet reduction*.

Contrary to the unitary dynamics \mathbb{U}_t , \mathbb{P} transforms pure states into mixtures thus increasing their von Neumann entropy; the process it describes is sometimes identified with a randomizing *quantum noise*, with decohering properties. By *decoherence* it is meant the result of any dynamical transformation that suppresses the phase-interferences present in a linear superposition of vector states.

Remark 2.3 The wave-packet reduction mechanism \mathbb{P} effectively describes what happens to S when it is not closed but in interaction with an external specific environment, in this case an apparatus measuring the observable X . Specifically, the wave packet reduction is the final effect on the open system S of its interaction with the macroscopic environment. \square

In the following, we shall be concerned with open quantum systems S immersed in an environment E . In principle, the environment should consist of infinitely many degrees of freedom and thus be addressed by means of the more proper algebraic approach to quantum statistical mechanics;^{37,38} however, for sake of clarity, we shall describe it by means of an infinite dimensional Hilbert space \mathfrak{H} and represent its states by density matrices ρ_E .^d

Subsystem S and environment E make a closed compound system $S + E$, its Hilbert space being the tensor product $\mathbb{C}^n \otimes \mathfrak{H}$; the total system evolves reversibly according to a group of dynamical maps $\mathbb{U}_t^{S+E} = \exp(t\mathbb{L}_{S+E})$ that act on the state-space $\mathcal{S}(S+E)$. The group is generated by formally exponentiating the commutator $\mathbb{L}_{S+E}[\rho_{S+E}] \equiv -i[H_{S+E}, \rho_{S+E}]$ with respect to a total Hamiltonian

$$H_{S+E} = H_S \otimes \mathbf{1}_E + \mathbf{1}_S \otimes H_E + \lambda H' , \quad (17)$$

where λ is an adimensional coupling constant, H' describes the $S - E$ interaction, while H_S and H_E are Hamiltonian operators pertaining to S , respectively E and $\mathbf{1}_{S,E}$ are identity operators. It follows that the generator decomposes as a sum of commutators,

$$\mathbb{L} \equiv \mathbb{L}_{S+E} = \mathbb{L}_S + \mathbb{L}_E + \lambda \mathbb{L}' , \quad (18)$$

where the subscripts S, E identify which degrees of freedom are involved.

Given a state $\rho_{S+E} \in \mathcal{S}(S+E)$ of the compound closed system, the statistical properties of the embedded subsystem S are described by a state $\rho_S \in \mathcal{S}(S)$ which is obtained by the *partial trace* over the degrees of freedom of E :

$$\mathcal{S}(S+E) \ni \rho_{S+E} \mapsto \rho_S \equiv \text{Tr}_E(\rho_{S+E}) = \sum_j \langle \psi_j^E | \rho_{S+E} | \psi_j^E \rangle , \quad (19)$$

where $\{|\psi_j^E\rangle\}$ is any orthonormal basis in \mathfrak{H} . The right hand side of (19) belongs to $M_n(\mathbb{C})$ and can be easily checked to be positive and normalized according to (3) and (2), so that $\rho_S \in \mathcal{S}(S)$.

Analogously, given any ρ_S at time $t = 0$, the state of S at any time t is

$$\rho_S(t) = \text{Tr}_E \left(\mathbb{U}_t^{S+E} [\rho_{S+E}] \right) . \quad (20)$$

This gives rise to a family of maps \mathbb{G}_t ,

$$\rho_S \mapsto \rho_S(t) = \mathbb{G}_t[\rho_S] , \quad (21)$$

^dAt a certain stage, one nevertheless has to perform the so-called thermodynamic limit, in which volume and number of degrees of freedom are let to infinity, while keeping the density finite. In practical terms, this amounts to substituting integrals for discrete summations, *e.g.* see Example 3.3.

which in general depend on ρ_S and can not be extended to the whole of the state-space. If we ask that \mathbb{G}_t preserve the convex structure of $\mathcal{S}(S)$, that is

$$\mathbb{G}_t \left[\sum_j \lambda_j \rho_S^j \right] = \sum_j \lambda_j \mathbb{G}_t \left[\rho_S^j \right], \quad (22)$$

then the initial state of the compound system must factorize: $\rho_{S+E} = \rho_S \otimes \rho_E$, where $\rho_S \in \mathcal{S}(S)$ and ρ_E is a fixed state of the environment.³⁹

The factorized form of the initial state means in particular that open system and environment are initially completely uncorrelated; though not true in general, in many interesting physical contexts such a condition is fully consistent and gives rise to a family of dynamical maps \mathbb{G}_t depending on the environment reference state ρ_E , but otherwise acting linearly on the state-space of S .^e

The family of maps \mathbb{G}_t , $t \geq 0$, describes a forward-in-time irreversible dynamics, for the partial trace breaks time-reversal; what the family lacks is a semigroup composition law, since in general $\mathbb{G}_t \circ \mathbb{G}_s \neq \mathbb{G}_{t+s}$ for $t, s \geq 0$. An equality would express the absence of cumulative memory effects, as such it is expected to be a good approximation of the time-evolution of open quantum systems only when their interaction with the environment is sufficiently weak or the environment time-correlations decay rapidly with respect to time-variation of the system.

The technical procedures to eliminate memory effects and recover semigroups of dynamical maps as reduced time-evolutions are known as *Markov approximations*. These will be discussed in detail in the next Section; in the remaining part of the present Section we shall study the structure of \mathbb{G}_t as a linear map, focusing on its physical properties.

2.2. Positivity and Complete Positivity

As motivated before, we take an initial state of the compound system $S + E$ in factorized form $\rho_{S+E} = \rho_S \otimes \rho_E$. By performing the partial trace with respect to the orthonormal basis of eigenvectors $|r_j^E\rangle$ of ρ_E with corresponding eigenvalues r_j^E , one obtains:^{1,34}

$$\begin{aligned} \rho_S(t) &= \text{Tr}_E \left(\mathbb{U}_t^{S+E} [\rho_S \otimes \rho_E] \right) = \sum_{j,k} r_k^E \langle r_j^E | U_t^{S+E} | r_k^E \rangle \rho_S \langle r_k^E | U_{-t}^{S+E} | r_j^E \rangle \\ &= \sum_{\alpha} \mathcal{V}_{\alpha}(t) \rho_S \mathcal{V}_{\alpha}^{\dagger}(t), \end{aligned} \quad (23)$$

where α is a double summation index and

$$\mathcal{V}_{\alpha}(t) \equiv \sqrt{r_k^E} \langle r_j^E | U_t^{S+E} | r_k^E \rangle. \quad (24)$$

^eAs already mentioned, in presence of initial correlations between subsystem and environment, a reduced dynamics that acts linearly on all $\mathcal{S}(S)$ can not in general be defined: its explicit form crucially depends also on the initial reduced state $\text{Tr}_E[\rho_{S+E}]$; for further investigations on this issue, see Refs.[40, 41, 7], and references therein.

The matrix elements $\langle r_j^E | U_t^{S+E} | r_k^E \rangle$ are elements of $M_n(\mathbb{C})$; further, from normalization ($\text{Tr}(\rho_S(t)) = 1$), it follows that

$$\sum_{\alpha} \mathcal{V}_{\alpha}^{\dagger}(t) \mathcal{V}_{\alpha}(t) = \mathbf{1}_n , \quad (25)$$

where $\mathbf{1}_n \in M_n(\mathbb{C})$ denotes the identity matrix.

The duality relation (13) associates to the linear map

$$\rho_S \mapsto \mathbb{G}_t[\rho_S] = \sum_{\alpha} \mathcal{V}_{\alpha}(t) \rho_S \mathcal{V}_{\alpha}^{\dagger}(t) , \quad (26)$$

on the state-space $\mathcal{S}(S)$, the dual action

$$X \mapsto \mathbb{G}_t^*[X] = \sum_{\alpha} \mathcal{V}_{\alpha}^{\dagger}(t) X \mathcal{V}_{\alpha}(t) , \quad (27)$$

on the algebra of observables $M_n(\mathbb{C})$. The latter fulfils $\mathbb{G}_t^*[\mathbf{1}_n] = \mathbf{1}_n$, a property called *unitality*.

The structure of both \mathbb{G}_t and \mathbb{G}_t^* is similar to the wave-packet reduction (16), with the difference that the $\mathcal{V}_{\alpha}(t)$ need not be orthogonal one-dimensional projectors as the P_i . By means of (3), it is easy to see that these linear maps preserve the positivity of operators: they belong to the class of *positive maps*.³⁵

Definition 2.2 *A linear map $\Lambda : M_n(\mathbb{C}) \mapsto M_n(\mathbb{C})$ is termed positive if it sends positive matrices into positive matrices, namely if*

$$0 \leq X \mapsto \Lambda[X] \geq 0 . \quad (28)$$

Remark 2.4 While positivity of hermitian matrices means positivity of their eigenvalues, positivity of linear maps means their property of transforming a matrix with positive eigenvalues into another such matrix. Positive linear maps are sometimes more properly referred to as positivity-preserving maps. \square

It turns out that linear maps as \mathbb{G}_t , \mathbb{G}_t^* and \mathbb{P} belong to a special subclass of positive maps on $M_n(\mathbb{C})$: the so-called *completely positive* maps.^{33,35}

Complete positivity is a stronger property than positivity. It concerns the possibility that the system S be statistically coupled to a so-called *ancilla*, A , that is to a generic remote and inert, finite-dimensional system. If A is m -dimensional, any linear map Λ on $M_n(\mathbb{C})$ lifts to a map $\Lambda \otimes \text{id}_A$ on the algebra $M_n(\mathbb{C}) \otimes M_m(\mathbb{C})$ of the compound system $S + A$, where id_A denotes the identical action on $M_m(\mathbb{C})$ leaving all operators unaffected. In the following the identical action will appear either as id_A or as id_m , explicitly indicating the dimensionality of the ancillary system.

The physical interpretation of such a coupling is as follows: the system S of interest may have interacted in the past with A and become correlated (entangled) with it; afterwards and prior to the start of the evolution of S , S and A has ceased to interact so that what is left are the statistical correlations between them incorporated in the state ρ_{S+A} . When the evolution (or more in general any state change)

of S sets in, it has to be considered as a transformation of the compound system $S + A$, which does not affect the ancilla and is thus mathematically described by the *lifting* $\Lambda \otimes \text{id}_A$ of the map Λ .

Definition 2.3 *A linear map $\Lambda : M_n(\mathbb{C}) \mapsto M_n(\mathbb{C})$ is completely positive, if and only if $\Lambda \otimes \text{id}_A$ is positive on $M_n(\mathbb{C}) \otimes M_m(\mathbb{C})$ for all $m \geq 1$, that is for all possible statistical couplings with finite-dimensional ancillas.*

When $m = 1$, $S + A$ is S itself as the Hilbert space $\mathbb{C}^n \otimes \mathbb{C}$ is isomorphic to \mathbb{C}^n . When $m \geq 2$, all elements of $M_n(\mathbb{C}) \otimes M_m(\mathbb{C})$ can be written as $m \times m$ $M_n(\mathbb{C})$ -valued matrices $[X_{ij}]_{i,j=1}^m$, $X_{ij} \in M_n(\mathbb{C})$; therefore, the definition concerns the linear actions $\Lambda \otimes \text{id}_A[[X_{ij}]] = [\Lambda[X_{ij}]]$ and selects among the positive linear maps Λ those such that⁴²

$$0 \leq \begin{pmatrix} X_{11} & \cdots & X_{1m} \\ \vdots & \ddots & \vdots \\ \vdots & \ddots & \vdots \\ X_{m1} & \cdots & X_{mm} \end{pmatrix} \xrightarrow{\Lambda \otimes \text{id}_A} \begin{pmatrix} \Lambda[X_{11}] & \cdots & \Lambda[X_{1m}] \\ \vdots & \ddots & \vdots \\ \vdots & \ddots & \vdots \\ \Lambda[X_{m1}] & \cdots & \Lambda[X_{mm}] \end{pmatrix} \geq 0 .$$

In the following Theorem, we recall two important results characterizing completely positive maps (see Refs.[42, 34, 33] for their proofs). The first one states that, in order to ascertain the complete positivity of $\Lambda : M_n(\mathbb{C}) \mapsto M_n(\mathbb{C})$, it is not necessary to check all dimensions m , while the second one establishes that complete positive Λ are exactly those with the same structure as \mathbb{U}_t , \mathbb{P} , \mathbb{G}_t and \mathbb{G}_t^* .

Theorem 2.1

- A linear map $\Lambda : M_n(\mathbb{C}) \mapsto M_n(\mathbb{C})$ is completely positive, if and only if $\Lambda \otimes \text{id}_n$ is positive on $M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$.
- A linear map $\Lambda : M_n(\mathbb{C}) \mapsto M_n(\mathbb{C})$ is completely positive, if and only if it is expressible in Kraus-Stinespring form

$$\Lambda[X] = \sum_{\alpha} \mathcal{V}_{\alpha}^{\dagger} X \mathcal{V}_{\alpha} , \quad (29)$$

where $\mathcal{V}_{\alpha} \in M_n(\mathbb{C})$ are such that $\sum_{\alpha} \mathcal{V}_{\alpha}^{\dagger} \mathcal{V}_{\alpha}$ converges (to $\mathbf{1}_n$ if Λ is unital).

Suppose one has a linear map on $M_n(\mathbb{C})$ given in the form

$$\Lambda[X] = \sum_{\alpha, \beta} C_{\alpha\beta} \mathcal{W}_{\alpha}^{\dagger} X \mathcal{W}_{\beta} , \quad (30)$$

with $\mathcal{W}_{\alpha} \in M_n(\mathbb{C})$ and $C_{\alpha\beta}$ making a hermitian matrix of coefficients such that $\sum_{\alpha, \beta} C_{\alpha\beta} \mathcal{W}_{\alpha}^{\dagger} \mathcal{W}_{\beta}$ converges. By diagonalizing $[C_{\alpha\beta}] = U^{\dagger} \text{diag}(d_1, d_2, \dots) U$, one recovers (29) if and only if $[C_{\alpha\beta}]$ is positive definite and the eigenvalues d_i positive; indeed, $C_{\alpha\beta} = \sum_j d_j U_{j\alpha}^* U_{j\beta}$ and this serves to redefine $\mathcal{V}_j = \sum_{\alpha} \sqrt{d_j} U_{j\alpha}^* \mathcal{W}_{\alpha}$.

Remark 2.5 If not all d_j are positive, then the map can be separated into two sums, one over the positive and the other over the negative eigenvalues; by extracting an overall minus sign, Λ can then be written as the difference of two completely positive maps $\Lambda_{1,2}$: $\Lambda = \Lambda_1 - \Lambda_2$. The property of complete positivity fixes the structure of the map by excluding the presence of a Λ_2 , while that of positivity is still far from being understood: no general prescriptions on $\Lambda_{1,2}$ are known that ensure the positivity of Λ . \square

Completely positive maps are a proper subset of all positive maps, for not all positive maps Λ lift to positive $\Lambda \otimes \text{id}_A$, the foremost example being the transposition.

Examples 2.1

(1) In $M_2(\mathbb{C})$, let $\mathbb{T}_2 : \begin{pmatrix} a & b \\ c & d \end{pmatrix} \mapsto \begin{pmatrix} a & c \\ b & d \end{pmatrix}$; the transposition map \mathbb{T}_2 does not alter the spectrum and therefore is a positive linear map. Let $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ be an orthonormal basis in \mathbb{C}^2 and consider the vector

$$|\Psi_+^{(2)}\rangle = \frac{1}{\sqrt{2}}(|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle) \in \mathbb{C}^2 \otimes \mathbb{C}^2.$$

The corresponding projection $P_+^{(2)} = |\Psi_+^{(2)}\rangle\langle\Psi_+^{(2)}| \in M_2(\mathbb{C}) \otimes M_2(\mathbb{C})$,

$$\begin{aligned} P_+^{(2)} &= \frac{1}{2} [|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1| + |0\rangle\langle 1| \otimes |0\rangle\langle 1| + |1\rangle\langle 0| \otimes |1\rangle\langle 0|] \\ &= \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}, \end{aligned} \tag{31}$$

has eigenvalues 0, 1 and gets transformed by $\mathbb{T}_2 \otimes \text{id}_2$ into

$$\begin{aligned} \mathbb{T}_2 \otimes \text{id}_2 [P_+^{(2)}] &= \frac{1}{2} (|0\rangle\langle 0| \otimes |0\rangle\langle 0| + |1\rangle\langle 1| \otimes |1\rangle\langle 1| \\ &\quad + |1\rangle\langle 0| \otimes |0\rangle\langle 1| + |0\rangle\langle 1| \otimes |1\rangle\langle 0|) \\ &= \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \end{aligned}$$

which has eigenvalues $\pm 1/2$ and is no longer a positive matrix. Therefore, \mathbb{T}_2 is positive, but not completely positive.

(2) The vector state $|\Psi_+^{(2)}\rangle$ generalizes to the totally symmetric state

$$|\Psi_+^{(n)}\rangle \equiv \frac{1}{\sqrt{n}} \sum_{j=1}^n |j\rangle \otimes |j\rangle \in \mathbb{C}^n \otimes \mathbb{C}^n, \quad (32)$$

where $|j\rangle$, $j = 1, 2, \dots, n$, is a reference orthonormal basis in \mathbb{C}^n . Then, with $P_+^{(n)} = |\Psi_+^{(n)}\rangle\langle\Psi_+^{(n)}|$, and \mathbb{T}_n the transposition on $M_n(\mathbb{C})$,

$$\mathbb{T}_n \otimes \text{id}_n[P_+^{(n)}] = \frac{1}{n} \sum_{j,k=1}^n |k\rangle\langle j| \otimes |j\rangle\langle k|,$$

and one checks that the sum in the right hand side of the second equality is the *flip operator* V on $\mathbb{C}^n \otimes \mathbb{C}^n$, such that $V(|\psi\rangle \otimes |\phi\rangle) = |\phi\rangle \otimes |\psi\rangle$, $\forall |\psi\rangle, |\phi\rangle \in \mathbb{C}^n$. It follows that V has eigenvalue -1 on any anti-symmetric state of $\mathbb{C}^n \otimes \mathbb{C}^n$ and thus the transposition is never completely positive in any dimension. \square

Remark 2.6 Transposition is associated with time-reversal;³⁷ as its lifting $\mathbb{T}_n \otimes \text{id}_n$ sends the state $P_+^{(n)}$ out of the space of states, it can not correspond to a physical operation. This means that time-reversal has to be applied globally and not locally, that is not on subsystems alone. \square

Examples 2.2 Let S be a quantum system described by a 2-dimensional Hilbert space \mathbb{C}^2 ; the algebra of observables $M_2(\mathbb{C})$ is linearly spanned by the identity matrix and the three Pauli matrices

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

namely, $X = \sum_{\mu=0}^3 X_\mu \sigma_\mu$ with $X_\mu = \frac{1}{2} \text{Tr}(X \sigma_\mu)$. The linear map

$$\mathbb{S}_\alpha : M_2(\mathbb{C}) \mapsto M_2(\mathbb{C}), \quad X \mapsto \mathbb{S}_\alpha[X] = \sigma_\alpha X \sigma_\alpha,$$

are written in the Kraus-Stinespring form (29), and are thus completely positive (although not unital).

(1) Consider the following two maps,

$$X \mapsto \frac{1}{2} \sum_{\alpha=0}^3 \mathbb{S}_\alpha[X], \quad X \mapsto \frac{1}{2} \sum_{\alpha=0}^3 \varepsilon_\alpha \mathbb{S}_\alpha[X], \quad (33)$$

where $\varepsilon_\alpha = 1$ when $\alpha \neq 2$, whereas $\varepsilon_2 = -1$. Using the algebraic relations

$$\sigma_\alpha \sigma_\beta \sigma_\alpha = \eta_{\alpha\beta} \sigma_\beta, \quad \text{where} \quad \eta_{\alpha\beta} =$$

$\beta \backslash \alpha$	0	1	2	3
0	1	1	1	1
1	1	1	-1	-1
2	1	-1	1	-1
3	1	-1	-1	1

it can be checked that the first map amounts to $X \mapsto \text{Tr}(X) \sigma_0$ and is completely positive since it is in Kraus-Stinespring form, while the second one is the transposition which indeed is such that $\mathbb{T}_2[\sigma_\alpha] = \varepsilon_\alpha \sigma_\alpha$, therefore positive, but not completely positive.

- (2) Given $\Lambda : M_2(\mathbb{C}) \mapsto M_2(\mathbb{C})$ in the form (30), by expanding the \mathcal{W}_α along the Pauli matrices σ_α it follows that the map can be rewritten as

$$X \mapsto \Lambda[X] = \sum_{\alpha, \beta=0}^3 C_{\alpha\beta} \sigma_\alpha X \sigma_\beta, \quad (34)$$

and is completely positive if and only if the matrix $[C_{\alpha\beta}]$ is positive definite. \square

The different structure of positive and completely positive maps on $M_n(\mathbb{C})$ is better exposed by means of the state $P_+^{(n)}$ of Example 2.1.2; one has:⁴³

Theorem 2.2

- $\Lambda : M_n(\mathbb{C}) \mapsto M_n(\mathbb{C})$ is positive if and only if

$$\langle \psi \otimes \phi | \Lambda \otimes \text{id}_n[P_+^{(n)}] | \psi \otimes \phi \rangle \geq 0, \quad \forall \psi, \phi \in \mathbb{C}^n. \quad (35)$$

- $\Lambda : M_n(\mathbb{C}) \mapsto M_n(\mathbb{C})$ is completely positive if and only if

$$\langle \Psi | \Lambda \otimes \text{id}_n[P_+^{(n)}] | \Psi \rangle \geq 0, \quad \forall \Psi \in \mathbb{C}^n \otimes \mathbb{C}^n. \quad (36)$$

The request in (36) is that the matrix $\Lambda \otimes \text{id}_n[P_+^{(n)}] \in M_{n^2}(\mathbb{C})$ be positive (see Definition 2.1), while the request in (35) involves mean values with respect to product vector states, only. These latter do not exhaust the Hilbert space, as there are non-product states as $|\Psi_+^{(n)}\rangle$.

2.3. Complete Positivity and Quantum Entanglement

The projector $P_+^{(n)}$ is the typical instance of an *entangled pure state*, the general notion of entanglement as opposed to that of *separability* being as follows.

Definition 2.4 Let $\mathcal{S}(S_1)$ and $\mathcal{S}(S_2)$ be the state-spaces of two n -level quantum systems $S_{1,2}$; within the state-space $\mathcal{S}(S_1 + S_2)$ one distinguishes the (convex) subset of separable states of the form

$$\rho_{S_1+S_2} = \sum_{ij} \lambda_{ij} \rho_i^1 \otimes \rho_j^2, \quad \lambda_{ij} \geq 0, \quad \sum_{ij} \lambda_{ij} = 1, \quad \rho_{i,j}^{1,2} \in \mathcal{S}(S_{1,2}). \quad (37)$$

All those states which can not be written as linear convex combinations of product states as in (37) are called *entangled*.

Remarks 2.7

- (1) The first two terms in the first line of (31) represent separable states: it is the presence of the remaining two interference terms that makes $P_+^{(2)}$ entangled.
- (2) It is often stated that while separable states only carry the classical correlations embodied in the weights λ_{ij} in (37), entangled states carry instead non-classical correlations, that is they are characterized by statistical properties which are not describable by classical probability theory. This is best seen by considering the projector $P_+^{(n)} = |\Psi_+^{(n)}\rangle\langle\Psi_+^{(n)}|$, its von Neumann entropy $S(P_+^{(n)}) = 0$. The partial trace of $P_+^{(n)}$ over either the first or the second system in $S + S$ gets the totally mixed state $\tau_n = \mathbf{1}_n/n$. This state has maximal entropy $S(\tau_n) = \log n$, despite S being a subsystem of $S + S$, which has zero entropy; instead, in classical probability theory, knowledge of the whole means having full information on all its parts. \square

At first glance one may think that the positivity of linear maps Λ on $\mathcal{S}(S)$ may be sufficient to guarantee a consistent description of all possible physical transformations of the states of S : after all, if a map Λ preserves the trace and the positivity of the spectrum of all density matrices, then it maps the state-space $\mathcal{S}(S)$ into itself as physical transformations surely do. In fact, a minimal consistency request is

Physically consistent transformations on $\mathcal{S}(S)$ must preserve the interpretation of the eigenvalues of all density matrices as probabilities and thus respect the positivity of their spectra.

One can now appreciate the important physical consequence of Theorem 2.2; indeed, from (35) and (36) it turns out that if $\Lambda : M_n(\mathbb{C}) \mapsto M_n(\mathbb{C})$ is positive, but not completely positive, then $\Lambda \otimes \text{id}_n[P_+^{(n)}]$ is *not* a positive matrix.

Given an n -dimensional ancilla A , statistically coupled to S , operating the transformation Λ on $\mathcal{S}(S)$ amounts to act with $\Lambda \otimes \text{id}_A$ on the state-space $\mathcal{S}(S + A)$ of the compound system $S + A$. Now, among the states of $S + A$, the totally symmetric projector $P_+^{(n)}$ is a physically plausible initial state, which is not transformed into a state by $\Lambda \otimes \text{id}_A$. For this to be true, Λ has to be completely positive. Positivity alone suffices for physical consistency on S , but not on $S + A$; in other words, positive maps can not properly describe physical transformations, only completely positive maps may do. Hence,

Complete positivity of maps is necessary to ensure their physical consistency against possible entanglement with ancillas

Remark 2.8 Admittedly, though logically stringent, the explanation of why consistent state-transformations must be completely positive is scarcely appealing from a physical point of view. Indeed, the ancilla system A is remote from S and inert; a more concrete scenario will be offered in Section 3.2 when we deal with dissipative time-evolutions. On the contrary, couplings to ancillas are natural tools in quantum

information, although, in this case, one deals with quantum channels and not with continuous time-evolutions. \square

If positive maps do not consistently describe physical transformations, they play however a fundamental role in the detection of entangled states. Due to the recent fast advances in quantum information theory, entanglement has turned from a quantum riddle with epistemological overtones into a practical physical resource that must be detected, quantified and manipulated. For instance, bipartite entangled pure states as $P_+^{(2)}$ are essential ingredients in quantum cryptography, quantum teleportation and quantum computation.¹⁸

2.3.1. Entanglement Detection

From Definition 2.4, entangled states can generically be mixed. While, it is easy to spot entangled pure states, it is much harder in the case of density matrices.

Example 2.3 As a first simple indication of these difficulties, consider the totally depolarized state of two 2-dimensional systems $\tau_2 = \mathbf{1}_4/4$. The identity matrix can be written in terms of the projectors onto the orthonormal basis of the so-called *Bell states*,

$$\tau_2 = \frac{1}{4} \left(P_+^{(2)} + P_-^{(2)} + Q_+^{(2)} + Q_-^{(2)} \right),$$

where $P_+^{(2)}$ is as in Example 2.1.1 while $P_-^{(2)} = |\Psi_-^{(2)}\rangle\langle\Psi_-^{(2)}|$, $Q_\pm^{(2)} = |\Phi_\pm^{(2)}\rangle\langle\Phi_\pm^{(2)}|$ and

$$|\Psi_-^{(2)}\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle), \quad |\Phi_\pm^{(2)}\rangle = \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle).$$

As a combination of entangled projectors, τ_2 may be deemed entangled. However, mixtures of entangled states have less entanglement than their constituents; indeed,

$$\tau_2 = \frac{1}{4} \left(|00\rangle\langle 00| + |01\rangle\langle 01| + |10\rangle\langle 10| + |11\rangle\langle 11| \right),$$

and thus, as a combination of separable states, τ_2 is indeed separable. \square

A substantial help in detecting entanglement comes from the transposition as defined in Examples 2.1, where one looked at the effects of the action of the transposition on only one of the factors of a bipartite system $S + S$, the so-called *partial transposition* $\mathbb{T}_n \otimes \text{id}_n$. Also, based on the fact that separable states make a closed convex subset of the state-space which can be geometrically separated from any given entangled state by a suitable (hyper) plane, one deduces the so-called *Peres-Horodecki criterion* for separability.⁴³

Theorem 2.3 *Let S be an n -dimensional system. Then,*

- *a state $\rho \in \mathcal{S}(S + S)$ is entangled if it does not remain positive under partial transposition $\mathbb{T}_n \otimes \text{id}_n$.*⁴⁴

More in general:

- a state $\rho \in \mathcal{S}(S + S)$ is entangled only if $\exists \Lambda : M_n(\mathbb{C}) \mapsto M_n(\mathbb{C})$ positive such that $\Lambda \otimes \text{id}_n[\rho]$ is not positive.⁴⁵

The sufficient condition easily follows from the fact that the action of any positive map Λ , lifted on separable states ρ_{sep} as in (37),

$$\Lambda \otimes \text{id}_n[\rho_{sep}] = \sum_{i,j} \lambda_{ij} \Lambda[\rho_i^1] \otimes \rho_j^2, \quad (38)$$

keeps their positivity, for Λ keeps the positivity of all $\rho^1 \in \mathcal{S}(S_1)$ by assumption. Therefore, if a positive map like the transposition, is such that once lifted it does not preserve the positivity of $\rho \in \mathcal{S}(S + S)$ then the state must be entangled: such a positive map is called an *entanglement detector* for ρ .

Of course, entanglement detectors can not be completely positive maps since, according to Definition 2.3, they are exactly those positive maps on $M_n(\mathbb{C})$ such that, once lifted to act on $M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$, they remain positive.

In line of principle, the transposition is a good entanglement detector for some states and not for others; one may thus suspect that, in general, all positive maps have to be checked in order to detect the entanglement of a generic ρ . Fortunately, in the case of a bipartite system consisting of two 2-level systems, or more in general of one 2-level and one 3-level system, the property of not remaining positive under partial transposition is also a necessary condition for their states to be entangled. In other words,⁴⁶

Theorem 2.4 *Consider a bipartite system $S_1 + S_2$, with S_1 a 2-level system and S_2 either a 2-level or a 3-level system; a state $\rho \in \mathcal{S}(S_1 + S_2)$ is entangled if and only if $\mathbb{T}_2 \otimes \text{id}_2[\rho]$, respectively $\mathbb{T}_2 \otimes \text{id}_3[\rho]$, is not positive.*

Example 2.4 Consider the $n^2 \times n^2$ matrix:

$$\rho_F = \alpha \mathbf{1}_n \otimes \mathbf{1}_n + \beta V \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C}), \quad \alpha, \beta \in \mathbb{R},$$

where V is the flip operator introduced in Example 2.1.2,

$$V = n \mathbb{T}_n \otimes \text{id}_n[P_+^{(n)}], \quad (39)$$

and the parameter F is defined by

$$F \equiv \text{Tr}[\rho_F V] = \alpha n + \beta n^2. \quad (40)$$

The second equality follows from the fact that $V^2 = \mathbf{1}_n \otimes \mathbf{1}_n$ and that, by choosing a basis $|i, j\rangle = |i\rangle \otimes |j\rangle \in \mathbb{C}^n \otimes \mathbb{C}^n$, then $V|i, j\rangle = |j, i\rangle$. We want ρ_F to be a density matrix. Since V has eigenvalues ± 1 , ρ_F has eigenvalues $\alpha \pm \beta$, positivity and normalization are guaranteed by

$$-\alpha \leq \beta \leq \alpha, \quad \text{Tr}(\rho_F) = \alpha n^2 + \beta n = 1. \quad (41)$$

Conditions (40) and (41) give

$$\alpha = \frac{n-F}{n(n^2-1)}, \quad \beta = \frac{nF-1}{n(n^2-1)}, \quad -1 \leq F \leq 1.$$

The states of the one-parameter family

$$\rho_F = \frac{n-F}{n(n^2-1)} \mathbf{1}_n \otimes \mathbf{1}_n + \frac{nF-1}{n(n^2-1)} V, \quad (42)$$

are called *Werner states*.⁴⁷ They are all and the only states that commute with all unitary transformation on $\mathbb{C}^n \otimes \mathbb{C}^n$ of the form $U \otimes U$ with U any unitary operator on \mathbb{C}^n . By performing the partial transposition on ρ_F , using (39) one gets

$$\mathbb{T}_n \otimes \text{id}_n[\rho_F] = \frac{n-F}{n(n^2-1)} \mathbf{1}_n \otimes \mathbf{1}_n + \frac{nF-1}{(n^2-1)} P_+^{(n)},$$

with an (n^2-1) -degenerate eigenvalue $\frac{n-F}{n(n^2-1)}$ which is never negative, and a nondegenerate eigenvalue

$$\frac{n-F}{n(n^2-1)} + \frac{nF-1}{(n^2-1)} = \frac{F}{n},$$

which is negative when $F < 0$. Therefore, in agreement with the preceding discussion, when $F < 0$, the Werner states are necessarily entangled, otherwise the partial transposition could not spoil the positivity of their spectrum.

It turns out that $F < 0$ is not only sufficient, but also necessary for ρ_F to be entangled:⁴⁷ in other words, ρ_F is separable if and only if $F \geq 0$. Since $F \geq 0$ means remaining positive under partial transposition, the latter is actually an exhaustive entanglement-detector relative to the family of Werner states also in dimension larger than two. \square

In the case of bipartite 2-dimensional systems, there exists a quantitative method to determine whether a state $\rho \in \mathcal{S}(S+S)$ is entangled or not, based on the notion of *concurrence*.^{48,49,50} This is defined as follows: with the tensor products of Pauli matrices $\sigma_2 \otimes \sigma_2$, one constructs

$$R \equiv \rho \sigma_2 \otimes \sigma_2 \rho^* \sigma_2 \otimes \sigma_2, \quad (43)$$

where ρ^* denotes ρ with complex-conjugated entries. The matrix R turns out to have positive eigenvalues; let R_i , $i = 1, 2, 3, 4$, be the positive square roots of its eigenvalues in decreasing order.

Theorem 2.5 *A state $\rho \in \mathcal{S}(S+S)$, with S two-dimensional, is entangled if and only if its concurrence*

$$\mathcal{C}(\rho) \equiv \max\{R_1 - R_2 - R_3 - R_4, 0\}, \quad (44)$$

is strictly positive.

Example 2.5 We consider the family of Werner states studied in the previous Example and set $n = 2$. Using the Bell states introduced in Example 2.3, the flip operator explicitly reads

$$V = P_+^{(2)} + P_-^{(2)} + Q_+^{(2)} - Q_-^{(2)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

whence

$$\rho_F = \frac{1}{6} \begin{pmatrix} 1+F & 0 & 0 & 0 \\ 0 & 2-F & 2F-1 & 0 \\ 0 & 2F-1 & 2-F & 0 \\ 0 & 0 & 0 & 1+F \end{pmatrix}.$$

Further, one checks that $\sigma_2 \otimes \sigma_2 \rho_F \sigma_2 \otimes \sigma_2 = \rho_F$; then (43) gives $R = \rho_F^2$; therefore, the eigenvalues R_i are $(1+F)/6$ (three times degenerate) and $(1-F)/2$, which are non-negative, since $-1 \leq F \leq 1$; thus, the difference $R_1 - R_2 - R_3 - R_4$ in (44) can assume only two expressions: $-F$ and $(F-2)/3$. As a consequence, the concurrence is $\mathcal{C}(\rho_F) = -F > 0$, if and only if $F < 0$, which, as already seen in the previous Example, is a necessary and sufficient condition for ρ_F to be entangled. \square

3. Reduced Dynamics and Markov Approximations

According to the previous considerations, the completely positive maps \mathbb{G}_t in (26) constitute a physically consistent description of the irreversible dynamics of a system S in interaction with its environment E . The only necessary assumption is that the initial state of $S + E$ do not carry either classical or quantum correlations and be of the form $\rho_S \otimes \rho_E$.

However, the dissipative and noisy effects due to E are hidden within the operators $\mathcal{V}_\alpha(t)$ and quite difficult to be read off; in particular, the one-parameter family of maps \mathbb{G}_t contains memory effects. On the other hand, if the interaction between S and E is sufficiently weak, one expects that, on a typical time-scale, the dynamics of S might be disentangled from that of the total system and efficiently described by a one-parameter semigroup of maps γ_t , $t \geq 0$, satisfying the forward in time composition law $\gamma_t \circ \gamma_s = \gamma_{t+s}$, $t, s \geq 0$.

The memory effects present in \mathbb{G}_t are best revealed by writing the formal integro-differential evolution equation of which the maps \mathbb{G}_t are solutions. Its standard derivation is via the so-called projection technique^f which we shall review in some detail by presenting and comparing several Markov approximations, leading to *master equations* of the form

$$\partial_t \rho_S(t) = (\mathbb{L}_H + \mathbb{D})[\rho_S(t)], \quad (45)$$

^fOriginally introduced in Refs.[51, 52], it is widely used in non-equilibrium statistical mechanics.⁵³

where \mathbb{L}_H acts on the state-space $\mathcal{S}(S)$ as $(-i$ times) the commutator with an effective Hamiltonian $H = H^\dagger \in M_n(\mathbb{C})$ as in (10), whereas \mathbb{D} is a linear operator on $\mathcal{S}(S)$, not in the form of a commutator, that effectively accounts for the dissipative and noisy effects due to E .

The solutions γ_t , $t \geq 0$, to (45) will describe the *reduced dynamics* of S as a semigroup of linear maps on $\mathcal{S}(S)$, obtained by exponentiating the generator:

$$\gamma_t = \exp \left[t \left(\mathbb{L}_H + \mathbb{D} \right) \right] . \quad (46)$$

The arguments developed in the previous sections about positivity and complete positivity lead to the conclusion that the latter property is necessary to ensure physical consistency against couplings to ancillas. Therefore, one can state in full generality that

any physically consistent Markovian approximation must yield semigroups γ_t consisting of completely positive maps.

In the following, we shall not abide by this request and expose the inconsistencies thereby arising; before this, however, we discuss the general form that time-continuous semigroups of completely positive maps must have.

3.1. Abstract Form of Generators of Dynamical Semigroups

Semigroups of the form (46) fulfill $\lim_{t \rightarrow 0} \gamma_t = \text{id}$; more precisely

$$\lim_{t \rightarrow 0} \|\gamma_t[\rho] - \rho\|_1 = 0, \forall \rho \in \mathcal{S}(S),$$

where $\|X\|_1 \equiv \text{Tr} \sqrt{X^\dagger X}$, $X \in M_n(\mathbb{C})$.

Time-continuity of a semigroup of maps γ_t guarantees the existence of a generator and an exponential structure as in (46).³³ We now proceed by imposing one by one those requests that are deemed necessary to physical consistency.^{1,2,3}

The first constraint is that the hermiticity of density matrices be preserved; we shall also ask for trace preservation. Physically speaking, this means that the overall probability is constant; in other words, we shall not be concerned with phenomena like particle decays that are characterized by loss of probability.^g

Interestingly, hermiticity and probability preservation suffice to partially fix the form of the generator.⁵⁴

Remark 3.1 Instead of directly referring to transformations on the state-space, the following theorem, as present in the literature, deals with semigroups γ_t^* acting

^gThese can nevertheless be included in the formalism: for instance, see Refs.[1, 25] and Remark 3.3.3 below.

on the algebra of observables $M_n(\mathbb{C})$ ($*$ denotes dual transformations on observables, namely in the Heisenberg picture). Hermiticity and trace preservation correspond to unitality, $\gamma_t^*[1] = 1$, and $(\gamma_t^*[X])^\dagger = \gamma_t^*[X^\dagger]$ for all $X \in M_n(\mathbb{C})$. Time-continuity is given with respect to the norm-topology: $\lim_{t \rightarrow 0} \|\gamma_t^*[X] - X\| = 0$, for all $X \in M_n(\mathbb{C})$, where

$$\|X\| = \sup \left\{ \sqrt{\langle \psi | X^\dagger X | \psi \rangle} , \|\psi\| = 1 \right\} .$$

Upon passing from the Heisenberg to the Schrödinger picture, one gets semigroups acting on states by means of the duality relation (13). \square

Theorem 3.1 *Let $\gamma_t^* : M_n(\mathbb{C}) \mapsto M_n(\mathbb{C})$, $t \geq 0$, form a time-continuous semigroup of unital, hermiticity-preserving linear maps. Then, the semigroup has the form $\gamma_t^* = \exp(t(\mathbb{L}_H^* + \mathbb{D}^*))$ with generator consisting of*

$$\mathbb{L}_H^*[X] = i[H, X] , \quad (47)$$

$$\mathbb{D}^*[X] = \sum_{i,j=1}^{n^2-1} C_{ij} \left(F_i X F_j^\dagger - \frac{1}{2} \{ F_i F_j^\dagger, X \} \right) , \quad (48)$$

where the matrix of coefficient C_{ij} (Kossakowski matrix) is hermitian, $H = H^\dagger$, and the F_j are such that $F_{n^2} = \mathbf{1}_n / \sqrt{n}$ and $\text{Tr}(F_j^\dagger F_k) = \delta_{jk}$, $0 \leq j, k \leq n^2$, while $\{, \}$ represents anticommutation.

The third constraint on γ_t^* is that they be positive maps, namely that they transform positive matrices into positive matrices. Indeed, as a consequence of the duality relation (13), the γ_t^* are positive maps if and only if their dual maps preserve the positivity of states $\rho \in \mathcal{S}(S)$; more precisely

$$0 \leq \text{Tr}(\gamma_t[\rho] X) \Leftrightarrow \text{Tr}(\rho \gamma_t^*[X]) \geq 0 .$$

It has been stressed that positivity preservation is necessary for physical consistency, but it is not sufficient against couplings with generic ancillas: for that the stronger request of complete positivity is compulsory.

The Hamiltonian contribution to the generator guarantees complete positivity since it gives rise to the standard unitary evolution \mathbb{U}_t that turns out to be automatically of the simplest Kraus-Stinespring form. Evidently, positivity and complete positivity both depend on the properties of the Kossakowski matrix C_{ij} .

Remark 3.2 Asking for positivity preservation results in quite an intricate algebraic problem; in fact, *no general necessary conditions*, but only sufficient ones are so far available on the coefficient C_{ij} such that they give rise to positivity preserving semigroups γ_t (for more details, see Refs.[56-59]). On the contrary, the condition that the γ_t be completely positive is far more stringent. \square

Theorem 3.2 *The semigroup $\{\gamma_t\}_{t \geq 0}$ consist of completely positive maps if and only if the Kossakowski matrix is positive definite.*

Remarks 3.3

- (1) The proof of Theorem 3.2 was given in Ref.[54] for finite-dimensional systems and in Ref.[55] in any dimension, under the assumption of boundedness of the generator. Generators with positive Kossakowski matrix are known as Kossakowski-Lindblad generators and the resulting semigroups are known as quantum dynamical semigroups.
- (2) Using the duality relation (13), one gets the following master equation on the state-space:

$$\mathbb{L}[\rho] = -i[H, \rho] + \sum_{i,j=1}^{d^2-1} C_{ij} \left(F_j^\dagger \rho F_i - \frac{1}{2} \{F_i F_j^\dagger, \rho\} \right). \quad (49)$$

The generated dual maps γ_t preserve the hermiticity and the trace of ρ ; if the Kossakowski matrix $[C_{ij}]$ is positive definite then $\gamma_t \otimes \text{id}_A$ preserves the positivity of all states of S and of the compound systems $S + A$ for any choice of finite-dimensional ancillas A .

- (3) By setting $K \equiv \sum_{i,j=1}^{d^2-1} C_{ij} F_i F_j^\dagger$, together with the Hamiltonian the anticommutator in (49) can be incorporated in a pseudo-commutator:

$$-i[H, \rho] - \frac{1}{2} \sum_{i,j=1}^{d^2-1} C_{ij} \{F_i F_j^\dagger, \rho\} = -i \left(H - \frac{i}{2} K \right) \rho + i \rho \left(H + \frac{i}{2} K \right).$$

The latter is the typical phenomenological expression for the generator of the time-evolution of a decaying system, where K describes loss of probability that is irreversibly transferred from the system S to the decay products.

- (4) Beside the pseudo commutator, the remaining contribution to dissipation comes from a term that, in the case of completely positive γ_t , can be put in Kraus-Stinespring form as done in (30). Such a term corresponds to what in classical Brownian motion is the diffusive effect of white-noise.¹⁷ It is of the form of the wave-packet reduction mechanism (16) and it is interpreted as quantum noise. \square

The consequences of the previous two theorems are best exposed in the two-dimensional setting as showed in the next example.

Example 3.1 Let $n = 2$ as in Examples 2.2; in such a case, by choosing the orthonormal basis of Pauli matrices $F_j = \sigma_j / \sqrt{2}$, $j = 1, 2, 3$, the dissipative contribution to the semigroup generator reads

$$\mathbb{D}[\rho] = \sum_{i,j=0}^3 C_{ij} \left(\sigma_j \rho \sigma_i - \frac{1}{2} \{ \sigma_i \sigma_j, \rho \} \right), \quad (50)$$

where a factor 1/2 has been absorbed into the coefficients C_{ij} . In the two-dimensional case, it proves convenient to adopt a vector-like representation; we

write density matrices in the form

$$\rho = \frac{1}{2}(\mathbf{1}_2 + \vec{\rho} \cdot \vec{\sigma}) = \frac{1}{2} \begin{pmatrix} 1 + \rho_3 & \rho_1 - i\rho_2 \\ \rho_1 + i\rho_2 & 1 - \rho_3 \end{pmatrix}, \quad 0 \leq \text{Det}[\rho] = \frac{1}{4} \left(1 - \sum_{j=1}^3 \rho_j^2\right), \quad (51)$$

where $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ and $\vec{\rho}$ is a vector in \mathbb{R}^3 , of unit length if and only if ρ is a pure state; it is usually referred to as the coherence¹ or Bloch⁸ vector. By representing ρ as a 4-vector $|\rho\rangle \equiv (1, \rho_1, \rho_2, \rho_3)$, any linear operation $\rho \mapsto \Lambda[\rho]$ corresponds to a 4×4 matrix $\mathcal{L} = [\mathcal{L}_{\mu\nu}]$ acting on $|\rho\rangle$. Thus, the evolution equation (45) can be recast in a Schrödinger-like form (the -2 in front is for sake of convenience)

$$\partial_t |\rho_t\rangle = -2(\mathcal{H} + \mathcal{D}) |\rho_t\rangle, \quad (52)$$

where the 4×4 matrices \mathcal{H} and \mathcal{D} correspond to the commutator \mathbb{L}_H and to the dissipative contribution \mathbb{D} .

It is no restriction to take the Hamiltonian of the form $H = \vec{\omega} \cdot \vec{\sigma}$, with $\omega_0 = 0$ and $\vec{\omega} = (\omega_1, \omega_2, \omega_3) \in \mathbb{R}^3$; using the algebraic relations $[\sigma_i, \sigma_j] = 2i \sum_{k=1}^3 \epsilon_{ijk} \sigma_k$, $i, j = 1, 2, 3$, it follows that

$$\mathcal{H} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \omega_3 & -\omega_2 \\ 0 & -\omega_3 & 0 & \omega_1 \\ 0 & \omega_2 & -\omega_1 & 0 \end{pmatrix}. \quad (53)$$

This is the typical anti-symmetric form of the action of commutators $-i[H, \cdot]$ when represented as a matrix acting on $|\rho\rangle$.

Concerning the dissipative matrix \mathcal{D} , the requests of trace and hermiticity preservation impose $\mathcal{D}_{0j} = 0$, $j = 1, 2, 3$, and $\mathcal{D}_{\mu\nu} \in \mathbb{R}$. By splitting \mathcal{D} into the sum of a symmetric and antisymmetric matrix, after incorporating the latter into \mathcal{H} , one remains with

$$\mathcal{D} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ u & a & b & c \\ v & b & \alpha & \beta \\ w & c & \beta & \gamma \end{pmatrix}, \quad (54)$$

where the nine real parameters depend on the phenomenology of the system-environment interaction. By exponentiation, one gets a semigroup of 4×4 matrices $\mathcal{G}_t = e^{-2t(\mathcal{H} + \mathcal{D})}$; its correspondence with the semigroup $\{\gamma_t\}_{t \geq 0}$ on the state-space $\mathcal{S}(S)$ is given by

$$\rho \mapsto \rho(t) = \gamma_t[\rho] = \sum_{\mu=0}^3 \rho_\mu(t) \sigma_\mu,$$

where $\rho_\mu(t)$ are the components of the 4-vector $|\rho_t\rangle$.

Since the trace is preserved at all times, checking positivity preservation amounts to checking whether $\text{Det}[\rho(t)] \geq 0$ for all $t \geq 0$ and for all initial ρ . The contributions

of the anti-symmetric \mathcal{H} cancel out, thus only the dissipative term remains and the time-derivative of the determinant reads

$$\dot{D}[\rho] \equiv \frac{d\text{Det}[\rho(t)]}{dt} \Big|_{t=0} = 2 \left[\sum_{i,j=1}^3 \mathcal{D}_{ij} \rho_i \rho_j + \sum_{j=1}^3 \mathcal{D}_{j0} \rho_j \right]. \quad (55)$$

Let ρ be a pure state: $P(\vec{n}) \equiv (\mathbf{1}_2 + \vec{n} \cdot \vec{\sigma})/2$, with \vec{n} a unit vector, $\|\vec{n}\| = 1$; then $\text{Det}[P(\vec{n})] = 0$. For positivity to be preserved, it is necessary that

$$\dot{D}[P(\vec{n})] = 2 \left(\sum_{i,j=1}^3 \mathcal{D}_{ij} n_i n_j + \sum_{j=1}^3 \mathcal{D}_{j0} n_j \right) \geq 0.$$

Sending $\vec{n} \mapsto -\vec{n}$, the same argument for the pure state $P(-\vec{n})$ yields

$$\dot{D}[P(-\vec{n})] = 2 \left(\sum_{i,j=1}^3 \mathcal{D}_{ij} n_i n_j - \sum_{j=1}^3 \mathcal{D}_{j0} n_j \right) \geq 0.$$

Summing the previous two inequalities and varying \vec{n} in the unit sphere, it turns out that positivity is preserved only if

$$\mathcal{D}^{(3)} = \begin{pmatrix} a & b & c \\ b & \alpha & \beta \\ c & \beta & \gamma \end{pmatrix} \geq 0. \quad (56)$$

The above condition on $\mathcal{D}^{(3)}$ is only necessary to positivity preservation as $\dot{D}[P(\vec{n})] < 0$ can follow because of the presence of the additional contribution $\sum_{j=1}^3 \mathcal{D}_{j0} \rho_j$. However, it becomes also sufficient when we ask that \mathcal{G}_t does not decrease the von Neumann entropy of any initial state, as this is equivalent to $u = v = w = 0$ in \mathcal{D} . Indeed, the totally depolarized state $\mathbf{1}_2/2$, *i.e.* $(1, 0, 0, 0)$ in vectorial notation, has maximal von Neumann entropy $\log 2$; if we impose that \mathcal{G}_t does not decrease its entropy, it can only stay constant, which means that $\mathbf{1}_2/2$ is a stationary state. In general, the vectorial expression of stationarity reads $(\mathcal{H} + \mathcal{D})|\rho\rangle = 0$, which in the case at hands implies $u = v = w = 0$.

In the following, we shall restrict to entropy-increasing semigroups; then, in terms of the entries C_{ij} , the matrix \mathcal{D} in (54) reads

$$\mathcal{D} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & C_{22} + C_{33} & -C_{12} & -C_{13} \\ 0 & -C_{12} & C_{11} + C_{33} & -C_{23} \\ 0 & -C_{13} & -C_{23} & C_{11} + C_{22} \end{pmatrix}. \quad (57)$$

Thus, the positivity of $[C_{ij}]$, which, according to the previous discussion, is necessary and sufficient for the complete positivity of γ_t , results in the inequalities

$$\begin{aligned} 2R &\equiv \alpha + \gamma - a \geq 0, & RS &\geq b^2, \\ 2S &\equiv a + \gamma - \alpha \geq 0, & RT &\geq c^2, \\ 2T &\equiv a + \alpha - \gamma \geq 0, & ST &\geq \beta^2, \\ RST &\geq 2bc\beta + R\beta^2 + Sc^2 + Tb^2. \end{aligned} \quad (58)$$

These constraints are much stronger than those coming from positivity alone, that is from $\mathcal{D}^{(3)} \geq 0$, which yields

$$\begin{cases} a \geq 0 \\ \alpha \geq 0 \\ \gamma \geq 0 \end{cases}, \quad \begin{cases} a\alpha \geq b^2 \\ a\gamma \geq c^2 \\ \alpha\gamma \geq \beta^2 \end{cases}, \quad \text{Det}\mathcal{D}^{(3)} \geq 0. \quad (59)$$

□

The fact that the conditions for complete positivity are stronger than those for positivity have an important physical consequence in that the decay-times related to dissipative completely positive semigroups must obey a definite hierarchy as showed in the following example.

Example 3.2 A typical relaxation behaviour induced by a heat bath on a two level system is determined by the following evolution equations for the entries ρ_{ij} of its density matrix:¹⁵

$$\frac{d\rho_{11}}{dt} = -p \rho_{11} + q \rho_{22}, \quad (60)$$

$$\frac{d\rho_{22}}{dt} = -q \rho_{22} + p \rho_{11}, \quad (61)$$

$$\frac{d\rho_{12}}{dt} = -(i\omega + r)\rho_{12}, \quad (62)$$

$$\frac{d\rho_{21}}{dt} = (i\omega - r)\rho_{21}, \quad (63)$$

where p, q, r and ω are positive constants, the latter representing the Hamiltonian contribution. The above time-evolution equations have been written for the standard matrix representation $\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix}$; going to the vectorial representation introduced in the previous example one gets

$$\partial_t |\rho_t\rangle = - \left[\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \omega & 0 \\ 0 & -\omega & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & r & 0 & 0 \\ 0 & 0 & r & 0 \\ p-q & 0 & 0 & p+q \end{pmatrix} \right] |\rho_t\rangle. \quad (64)$$

The choice $p = q$ induces entropy-increase, so that positivity-preservation is equivalent to the positivity of $\mathcal{D}^{(3)}$ which only requires $r, p \geq 0$. On the contrary, from (58), complete positivity asks for $r \geq p$, *i.e.* the so-called *phase-relaxation* $1/T_2 \equiv r$ must be larger or equal than $1/(2T_1)$, where $1/T_1$ is the so-called *population-relaxation*. □

Remark 3.4 The hierarchy between characteristic decay times induced by the request of complete positivity is often refused or challenged in the physical literature (*e.g.* see Refs.[39, 60-66]). Indeed, as already stressed, it arises because of the possibility of an uncontrollable statistical coupling of the experimentally accessible

system with an inert entity, the ancilla. Such abstract eventuality seems to be too weak to constrain the physical properties of dissipative quantum systems. We shall later show how the true role of complete positivity is far from being an abstract mathematical non-sense, but has to do with the possibility of entangled bi-partite states evolving dissipatively in a same environment. \square

3.2. Master Equation

In this Section, we describe how from the global time-evolution equation

$$\partial_t \rho_{S+E}(t) = \mathbb{L}_{S+E}[\rho_{S+E}(t)] , \quad (65)$$

by performing certain Markov approximations, one can obtain master equations as in (45).^{1,2,3} We shall be particularly interested in comparing them with the general form in (49).

The first step consists in defining a projection $P : \mathcal{S}(S+E) \mapsto \mathcal{S}(S+E)$ on the state-space of $S+E$ which, by partial tracing, extracts the state of S :

$$P[\rho_{S+E}] = \text{Tr}_E(\rho_{S+E}) \otimes \rho_E , \quad (66)$$

where ρ_E is a chosen environment reference state. It follows that $P^2 \equiv P \circ P = P$ and, with Q such that $P + Q = \mathbf{1}_{S+E}$,

$$P[\rho_S \otimes \rho_E] = \rho_S \otimes \rho_E , \quad Q[\rho_S \otimes \rho_E] = 0 . \quad (67)$$

The second step uses P and Q to split the evolution equation into the two coupled equations

$$\partial_t P[\rho_{S+E}(t)] = \mathbb{L}_{S+E}^{PP}[P[\rho_{S+E}(t)]] + \mathbb{L}_{S+E}^{PQ}[Q[\rho_{S+E}(t)]] , \quad (68)$$

$$\partial_t Q[\rho_{S+E}(t)] = \mathbb{L}_{S+E}^{QP}[P[\rho_{S+E}(t)]] + \mathbb{L}_{S+E}^{QQ}[Q[\rho_{S+E}(t)]] , \quad (69)$$

where $\mathbb{L}_{S+E}^{PP} \equiv P \circ \mathbb{L}_{S+E} \circ P$, $\mathbb{L}_{S+E}^{PQ} \equiv P \circ \mathbb{L}_{S+E} \circ Q$, $\mathbb{L}_{S+E}^{QQ} \equiv Q \circ \mathbb{L}_{S+E} \circ Q$ and $\mathbb{L}_{S+E}^{QP} \equiv Q \circ \mathbb{L}_{S+E} \circ P$.

Formal integration of the second equation yields:

$$Q[\rho_{S+E}(t)] = e^{t \mathbb{L}_{S+E}^{QQ}}[Q[\rho_{S+E}(0)]] + \int_0^t ds e^{(t-s) \mathbb{L}_{S+E}^{QQ}} \circ \mathbb{L}_{S+E}^{QP}[P[\rho_{S+E}(s)]] . \quad (70)$$

We shall now assume an uncorrelated initial state of the tensor product form $\rho_S \otimes \rho_E$. Thus, the first term on the right hand side vanishes because of (67); once inserted into (68), the solution (70) leads to the following evolution equation

$$\partial_t \rho_S(t) \otimes \rho_E = \mathbb{L}_{S+E}^{PP}[\rho_S(t) \otimes \rho_E] + \int_0^t ds \mathbb{L}_{S+E}^{PQ} \circ e^{(t-s) \mathbb{L}_{S+E}^{QQ}} \circ \mathbb{L}_{S+E}^{QP}[\rho_S(s) \otimes \rho_E] . \quad (71)$$

The tensorized ρ_E on the left hand side also appears on the right hand side because of (67)–(69); it can thus be traced away yielding a master equation for $\rho_S(t) \equiv \text{Tr}_E[\rho_{S+E}(t)]$.

At this point, one assumes the reference state ρ_E to be an equilibrium state of the dynamics of the environment alone,

$$\mathbb{L}_E[\rho_E] = -i[H_E, \rho_E] = 0. \quad (72)$$

Such a condition is physically plausible because typical environments are modelled as very large heat baths or thermostats whose equilibrium states are not perturbed by the interaction with S . As a consequence, $(\mathbf{1}_S \otimes \mathbb{L}_E)P = 0$; similarly, $P(\mathbf{1}_S \otimes \mathbb{L}_E) = 0$ follows from the cyclicity of the trace operation and expresses the conservation of probability in the environment.

Further, in (17), one assumes an interaction Hamiltonian of the form

$$\tilde{H}' = \sum_{\alpha} V_{\alpha} \otimes \tilde{B}_{\alpha}, \quad (73)$$

where V_{α} and \tilde{B}_{α} are hermitian operators acting on the Hilbert spaces \mathbb{C}^n of S , respectively \mathfrak{H} of E . It proves convenient to define *centered environment operators* $B_{\alpha} \equiv \tilde{B}_{\alpha} - \text{Tr}_E(\tilde{B}_{\alpha})$; in this way one gets a new Hamiltonian for S and a new interaction term

$$H_S^{\lambda} = H_S + \lambda \underbrace{\sum_{\alpha} V_{\alpha} \text{Tr}_E(\tilde{B}_{\alpha})}_{H_S^{(1)}}, \quad H' = \sum_{\alpha} V_{\alpha} \otimes B_{\alpha}, \quad \text{Tr}[\rho_E B_{\alpha}] = 0. \quad (74)$$

Remark 3.5 The redefinition of H_S amounts to a Lamb shift of the energy levels due to a mean-field, first order (in λ) approximation of the interaction with E . \square

Denoting by \mathbb{L}_S^{λ} ($-i$ times) the commutator with respect to H_S^{λ} and by \mathbb{L}' ($-i$ times) the commutator with respect to the new interaction term H' , the total Liouvillian in (65) becomes

$$\mathbb{L} \equiv \mathbb{L}_{S+E} = \mathbb{L}_S^{\lambda} \otimes \mathbf{1}_E + \mathbf{1}_S \otimes \mathbb{L}_E + \lambda \mathbb{L}'.$$

Moreover, by means of (72) and of the last relation in (74) one gets

$$P \circ (\mathbb{L}_S^{\lambda} \otimes \mathbf{1}_E) = (\mathbb{L}_S^{\lambda} \otimes \mathbf{1}_E) \circ P, \quad P \circ \mathbb{L}' \circ P = 0. \quad (75)$$

Using the latter relations and computing the partial trace Tr_E with respect to the orthonormal basis of eigenvectors of ρ_E , further yield

$$\mathbb{L}_{S+E}^{PP}[\rho_S(t) \otimes \rho_E] = (\mathbb{L}_S^{\lambda} \otimes \mathbf{1}_E)^{PP}[\rho_S(t) \otimes \rho_E] = \mathbb{L}_S^{\lambda}[\rho_S(t)] \otimes \rho_E, \quad (76)$$

$$\mathbb{L}_{S+E}^{PQ}[\rho_{S+E}(t)] = \lambda (\mathbb{L}')^{PQ}[\rho_{S+E}(t)] = \lambda \text{Tr}_E(\mathbb{L}' \circ Q[\rho_{S+E}(t)]) \otimes \rho_E, \quad (77)$$

$$\mathbb{L}_{S+E}^{QP}[\rho_S(t) \otimes \rho_E] = \lambda (\mathbb{L}')^{QP}[\rho_S(t) \otimes \rho_E] = \lambda \mathbb{L}'[\rho_S(t) \otimes \rho_E], \quad (78)$$

where the last equality follows from

$$Q \mathbb{L}'[\rho_S \otimes \rho_E] = \mathbb{L}'[\rho_S \otimes \rho_E] . \quad (79)$$

Inserting these expressions into (71) and getting rid of the appended factor ρ_E , one finally gets the *master equation*

$$\partial_t \rho_S(t) = \mathbb{L}_S^\lambda[\rho_S(t)] + \lambda^2 \int_0^t ds \operatorname{Tr}_E \left(\mathbb{L}' \circ e^{(t-s)\mathbb{L}^{QQ}} \circ \mathbb{L}'[\rho_S(s) \otimes \rho_E] \right) . \quad (80)$$

The second term in the right hand side of (80) compactly comprises the effects due to the environment; these are described by two nested commutators with respect to the interaction Hamiltonian H' , with the full time-evolution present in $\exp((t-s)\mathbb{L}^{QQ})$, and through a final overall trace over the environment degrees of freedom. Finding the concrete form of these effects would require the solution of the time-evolution of the total system $S + E$.

In order to proceed to a more manageable equation and to the elimination of all memory effects, one first notices that Tr_E makes the dissipative term ultimately depend on two-point correlation functions of the environment operators B_α . Memory effects are thus expected to become negligible on a time-scale much longer than the typical decay time τ_E of correlations in the environment.

That indeed this is the case can be illustrated with the help of the following simple, exactly solvable model of system-environment coupling.⁶⁷

Example 3.3 In the notation of Example 3.1, consider a two-level system immersed in a bosonic thermal bath at inverse temperature $\beta = T^{-1}$. The Hamiltonian for the total system contains three contributions as in (17):

$$H = \underbrace{\frac{\Omega}{2} \sigma_3 \otimes \mathbf{1}_E + \mathbf{1}_S \otimes}_{H_S} \underbrace{\sum_k \omega_k a_k^\dagger a_k}_{H_E} + \underbrace{\sigma_3 \otimes \sum_k \left(\lambda_k a_k^\dagger + \bar{\lambda}_k a_k \right)}_{H'} , \quad (81)$$

where, for simplicity, the bath modes are assumed to be one-dimensional. The first two pieces, giving together the free Hamiltonian H_0 , drive the uncoupled motion: Ω represents the splitting between the two system levels, while ω_k the energy of the bath modes, labelled by the discrete index k (the bath is for the moment assumed to be confined in a finite “box”); the corresponding creation, a_k^\dagger , and annihilation, a_k , operators are taken to satisfy the standard oscillator algebra: $[a_k^\dagger, a_{k'}] = \delta_{k,k'}$, $[a_k^\dagger, a_{k'}^\dagger] = [a_k, a_{k'}] = 0$.

The coupling between the subsystem and the bath degrees of freedom is described by the third contribution in (81), with λ_k , $\bar{\lambda}_k$ playing the role of mode-dependent coupling constants. Note that the interaction Hamiltonian H' is diagonal in the subsystem Hilbert space: it is this property that allows deriving an exact analytic expression for the total evolution operator $U_t = e^{-itH}$.

In order to get rid of the free motion, it is convenient to work in the interaction picture. Then, after conjugation with the free evolution operator $U_t^{(0)} = e^{-itH_0}$,

U_t can be obtained through the time-ordered exponentiation of the following time-dependent interaction Hamiltonian:

$$H'(t) = \sum_k \left[\lambda_k e^{i\omega_k t} A_k^\dagger + \bar{\lambda}_k e^{-i\omega_k t} A_k \right] \equiv \sum_k H'_k(t) . \quad (82)$$

Since the operators $A_k^\dagger \equiv \sigma_3 \otimes a_k^\dagger$, $A_k \equiv \sigma_3 \otimes a_k$ obey the same algebra as a_k^\dagger , a_k , this exponentiation can be computed in closed form using standard Lie algebraic manipulations.^{8,14} As a result, the time-evolution operator in the interaction picture reads (\mathcal{T} represents time ordering):

$$\begin{aligned} U(t_0, t) &\equiv \mathcal{T} e^{-i \int_{t_0}^t d\tau H'(\tau)} = \Pi_k \mathcal{T} e^{-i \int_{t_0}^t d\tau H'_k(\tau)} \\ &= e^{i\varphi(t-t_0)} \Pi_k e^{-i \int_{t_0}^t d\tau H'_k(\tau)} = e^{i\varphi(t-t_0)} e^{\sigma_3 \otimes K(t_0, t)} , \end{aligned} \quad (83)$$

where

$$\begin{aligned} \varphi(t-t_0) &= \sum_k \frac{|\lambda_k|^2}{\omega_k^2} \left[\omega_k(t-t_0) - \sin \omega_k(t-t_0) \right] , \\ K(t_0, t) &= \sum_k \left[f_k(t_0, t) a_k^\dagger - \bar{f}_k(t_0, t) a_k \right] , \end{aligned} \quad (84)$$

and

$$f_k(t_0, t) = -i \int_{t_0}^t d\tau \lambda_k e^{i\omega_k \tau} = \frac{\lambda_k}{\omega_k} \left(e^{i\omega_k t_0} - e^{i\omega_k t} \right) . \quad (85)$$

At the initial time t_0 , subsystem and environment are assumed to be uncorrelated, with the bath in a thermal equilibrium state described by the density matrix $\rho_E = e^{-\beta H_E} / \text{Tr}[e^{-\beta H_E}]$. The evolution in time of the reduced density matrix $\rho(t)$ pertaining to the subsystem is then given by:

$$\rho(t_0) \rightarrow \rho(t) = \text{Tr}_E \left[U(t_0, t) \rho(t_0) \otimes \rho_E U^\dagger(t_0, t) \right] . \quad (86)$$

A convenient basis in the two-dimensional subsystem Hilbert space is provided by the eigenvectors of H_S , $\sigma_3|i\rangle = (-1)^{i+1}|i\rangle$, $i = 0, 1$. Using (83), from (86) one then deduces the evolution of the corresponding matrix elements $\rho_{ij}(t) = \langle i|\rho(t)|j\rangle$:

$$\begin{aligned} \rho_{00}(t) &= \rho_{00}(t_0) , \quad \rho_{11}(t) = \rho_{11}(t_0) , \\ \rho_{10}(t) &= \text{Tr}_E \left[e^{2K(t_0, t)} \rho_E \right] \rho_{10}(t_0) = e^{-\Gamma(t_0, t)} \rho_{10}(t_0) , \end{aligned} \quad (87)$$

with

$$\Gamma(t_0, t) = 4 \sum_k \frac{|\lambda_k|^2}{\omega_k^2} \left[1 - \cos \omega_k(t-t_0) \right] \coth \left(\frac{\beta \omega_k}{2} \right) . \quad (88)$$

Only the off-diagonal matrix elements are affected by the interaction with the bath: in this case, the environment is responsible for the loss of quantum coherence, without affecting the population of the two levels; this is a consequence of the form of interaction Hamiltonian H' , which is diagonal in the chosen system basis.

In order to analyze in detail this decoherence phenomenon, it is useful to pass to the thermodynamical limit of the bath system: in this way, the mode label k becomes a continuous variable. The damping function (88) can then be expressed as an integral over the frequency variable ($\sum_k \rightarrow (1/2\pi) \int_0^\infty d\omega$):

$$\Gamma(t_0, t) \equiv \Gamma(t - t_0) = \frac{2\lambda^2}{\pi} \int_0^\infty d\omega \left[\frac{1 - \cos \omega(t - t_0)}{\omega} \right] \coth \left(\frac{\beta\omega}{2} \right) e^{-\varepsilon\omega}, \quad (89)$$

where a typical $\sqrt{\omega}$ dependence of the coupling constants on frequency has been assumed, together with a massless dispersion relation. The introduction of the damping exponential term is necessary to make the integral converge at infinity: physically, it is justified by assuming the presence of a characteristic scale $1/\varepsilon$ below which the system-bath coupling decreases rapidly, as found in many realistic models.

The function in (89) can be conveniently split as $\Gamma(t) = \Gamma_0(t) + \Gamma_\beta(t)$ into a vacuum, $\Gamma_0(t)$, and thermal, $\Gamma_\beta(t)$, contributions, that can be separately evaluated. The vacuum piece,

$$\Gamma_0(t) \equiv \frac{2\lambda^2}{\pi} \int_0^\infty d\omega \left[\frac{1 - \cos \omega t}{\omega} \right] \left[\coth \left(\frac{\beta\omega}{2} \right) - 1 \right] e^{-\varepsilon\omega} = \frac{\lambda^2}{\pi} \ln \left[1 + (t/\varepsilon) \right], \quad (90)$$

is temperature independent and describes how the bath vacuum fluctuations affect the quantum coherence of the two-level system. On the other hand, the action of the bath thermal fluctuations on the subsystem dynamics is determined by⁶⁸

$$\Gamma_\beta(t) \equiv \frac{4\lambda^2}{\pi} \int_0^t ds \int_0^\infty d\omega \sin \omega t \frac{e^{-\varepsilon\omega}}{e^{\beta\omega} - 1} = -\frac{4\lambda^2}{\pi} \ln \left[\frac{|\Gamma(1 + \varepsilon/\beta + it/\beta)|}{\Gamma(1 + \varepsilon/\beta)} \right]. \quad (91)$$

The existence in the problem of different time scales allows to identify, through the explicit results (90) and (91), three time regimes in the two-level system dynamics:

- (1) short times, $t \ll \varepsilon$, for which $\Gamma(t) \sim (\lambda^2/\pi)(t/\varepsilon)^2$; in this case the bath fluctuations hardly affect the subsystem free evolution;
- (2) intermediate times, $\varepsilon < t < \beta$, where $\Gamma(t) \sim (2\lambda^2/\pi) \ln(t/\varepsilon)$; here the main cause of decoherence is due to the vacuum fluctuations;
- (3) long time regime $t \gg \beta$, where $\Gamma(t) \sim (2\lambda^2/\beta)t$.^h This is the Markovian regime, which holds for times much longer than the characteristic decay time of the bath correlations, which is proportional to the inverse temperature, $\tau_E \simeq \beta$. The loss of coherence follows an exponential decreasing law, with a lifetime $T_2 = \beta/2\lambda^2$; this corresponds exactly to the phase relaxation parameter introduced in Example 3.2. As already mentioned, the population relaxation parameter T_1 is here vanishing due to the particularly simple choice of subsystem-bath coupling.

□

^hThis result follows from the following asymptotic behaviour of the modulus of $\Gamma(x + iy)$ as $|y| \rightarrow \infty$, for x and y real: $|\Gamma(x + iy)| \sim \sqrt{2\pi} |y|^{x-1/2} e^{-\pi|y|/2}$.⁶⁹

3.3. Markovian Approximations

Obtaining a physically consistent Markovian approximation for the master equation in (80) is notoriously tricky.^{1,2,3,70} Indeed, with respect to the previous Example, the situation is complicated by the dynamics of the system S alone, generated by the Hamiltonian H_S , which in general does not commute with the interaction with the bath. This introduces in the problem another timescale τ_S , and the need of a hierarchy condition $\tau_E \ll \tau_S$, that allow a clear separation between subsystem and environment. Following Ref.[71], we shall now present the most commonly used Markovian limits of (80), focusing in particular on their physical consistency, especially in relation to the property of complete positivity.

3.3.1. Second Order Approximation

One of the most simple assumptions allowing an immediate identification of subsystem and environment is the hypothesis of *weak coupling* between the two. In this case, the ratio τ_E/τ_S is small because $\tau_S \rightarrow \infty$, while τ_E remains finite, and further $\lambda \ll 1$. The master equation (80) can be more explicitly rewritten as

$$\begin{aligned} \partial_t \rho_S(t) = & -i \left[H_S + \lambda H_S^{(1)}, \rho_S(t) \right] \\ & - \lambda^2 \int_0^t ds \operatorname{Tr}_E \left(\left[H', e^{(t-s)\mathbb{L}_{S+E}^{QQ}} \left[H', \rho_S(s) \otimes \rho_E \right] \right] \right), \end{aligned} \quad (92)$$

making clear that dissipation becomes relevant on a *slow time-scale* of order λ^{-2} .

A first Markovian approximation to (92) can be euristically obtained as follows; integration of (92) yields:

$$\begin{aligned} \rho_S(t) = & e^{t\mathbb{L}_S^\lambda} [\rho_S(0)] - \lambda^2 \int_0^t dv \int_0^v du e^{(t-v)\mathbb{L}_S^\lambda} \times \\ & \times \operatorname{Tr}_E \left(\left[H', e^{(v-u)\mathbb{L}_{S+E}^{QQ}} \left[H', \rho_S(u) \otimes \rho_E \right] \right] \right). \end{aligned} \quad (93)$$

Then, by changing the integration order and by introducing the new integration variable $w \equiv v - u$, (93) becomes:

$$\begin{aligned} \rho_S(t) = & e^{t\mathbb{L}_S^\lambda} [\rho_S(0)] - \lambda^2 \int_0^t du e^{(t-u)\mathbb{L}_S^\lambda} \times \\ & \times \left\{ \int_0^{t-u} dw e^{-w\mathbb{L}_S^\lambda} \operatorname{Tr}_E \left(\left[H', e^{w\mathbb{L}_{S+E}^{QQ}} \left[H', \rho_S(u) \otimes \rho_E \right] \right] \right) \right\}. \end{aligned} \quad (94)$$

In view of the assumed smallness of the coupling constant λ , the dissipative character of the dynamics emerges on the slow time scale $\tau = \lambda^2 t$. A first instance of Markovian approximation consists in 1) substituting τ/λ^2 for t in the curly bracket and 2) in letting $\lambda \rightarrow 0$ in the upper limit of the integration in w and in the generators \mathbb{L}_S^λ and \mathbb{L}_{S+E} . As $\mathbb{L}_{S,E}$ commute with Q and because of (79), this

finally gets

$$\begin{aligned} \rho_S(t) = & e^{t\mathbb{L}_S^\lambda}[\rho_S(0)] - \lambda^2 \int_0^t du e^{(t-u)\mathbb{L}_S^\lambda} \times \\ & \times \int_0^\infty dw \operatorname{Tr}_E \left(e^{-w\mathbb{L}_S} \left[H', e^{w(\mathbb{L}_{HS} + \mathbb{L}_E)} \left[H', \rho_S(u) \otimes \rho_E \right] \right] \right), \end{aligned} \quad (95)$$

which is the formal solution to

$$\partial_t \rho_S(t) = -i \left[H_S + \lambda H_S^{(1)}, \rho_S(t) \right] + \lambda^2 \mathbb{D}_1[\rho_S(t)], \quad (96)$$

where

$$\mathbb{D}_1[\rho_S] = - \int_0^\infty ds \operatorname{Tr}_E \left(e^{-s\mathbb{L}_{HS}} \left[H', e^{s(\mathbb{L}_S + \mathbb{L}_E)} \left[H', \rho_S \otimes \rho_E \right] \right] \right). \quad (97)$$

Master equations of the form (96) with the dissipative contribution as in (97) are known as *Redfield equations*.¹⁵ Given the form (74) of the $S - E$ interaction, we set

$$V_\alpha(t) \equiv e^{-t\mathbb{L}_S} [V_\alpha] = e^{itH_S} V_\alpha e^{-itH_S}, \quad B_\alpha(t) \equiv e^{-t\mathbb{L}_E} [B_\alpha] = e^{itH_E} B_\alpha e^{-itH_E}. \quad (98)$$

Further, we introduce the environment *two-point correlation functions*

$$G_{\alpha\beta}(s) \equiv \operatorname{Tr} \left[\rho_E B_\alpha(s) B_\beta \right] = \operatorname{Tr} \left[\rho_E B_\alpha B_\beta(-s) \right]. \quad (99)$$

The dissipative term $\mathbb{D}_1[\rho_S(t)]$ exhibits the following structure of the environment induced second order effects:

$$\begin{aligned} \mathbb{D}_1[\rho_S(t)] = & - \sum_{\alpha,\beta} \int_0^\infty ds \left\{ G_{\alpha\beta}(s) \left[V_\alpha(s), V_\beta \rho_S(t) \right] \right. \\ & \left. + G_{\beta\alpha}(-s) \left[\rho_S(t) V_\beta, V_\alpha(s) \right] \right\}. \end{aligned} \quad (100)$$

In order to compare them with the Kossakowski-Lindblad generator (49), it is convenient to introduce the operators

$$C_\beta^S \equiv \sum_\alpha \int_0^\infty ds G_{\alpha\beta}(s) V_\alpha(s), \quad (101)$$

and rewrite

$$\begin{aligned} \mathbb{D}_1[\rho_S(t)] = & \sum_\beta \left\{ B_\beta^S \rho_S(t) C_\beta^S + (C_\beta^S)^\dagger \rho_S(t) B_\beta^S \right. \\ & \left. - C_\beta^S B_\beta^S \rho_S(t) - \rho_S(t) B_\beta^S (C_\beta^S)^\dagger \right\}. \end{aligned} \quad (102)$$

It can be verified that trace and hermiticity are preserved, namely that $\operatorname{Tr}(\mathbb{D}_1[\rho_S(t)]) = 0$ and that $(\mathbb{D}_1[\rho_S(t)])^\dagger = \mathbb{D}_1[\rho_S(t)]$. Despite a certain similarity to (49), in order to check whether the semigroup generated by the Redfield equations consists of completely positive maps one has to extract from (102) the corresponding Kossakowski matrix and ensure its positivity. Instead of doing this,

in the following example we shall show that, in general, the semigroups generated by the Redfield equations do not even preserve positivity.

Up to this point we have considered any equilibrium environment state ρ_E ; however, typical environments are heat baths and ρ_E thermal states at inverse temperature $\beta \equiv T^{-1}$. They satisfy the so-called *Kubo-Martin-Schwinger (KMS) conditions*³⁷

$$G_{\alpha\beta}(t) = G_{\beta\alpha}(-t - i\beta) . \quad (103)$$

These equalities express the analyticity properties of thermal correlation functions with respect to time; they are easily derived when H_E has discrete spectrum, but survive the thermodynamical limit and then hold for truly infinite environments.

Example 3.4 As in the previous Example, consider a two-level system immersed into a free Bose-gas in equilibrium at temperature $T = \beta^{-1}$. This time, however, we choose an interaction Hamiltonian which does not commute with the system one:

$$H_{S+E} = \underbrace{\frac{\Omega}{2}\sigma_3 \otimes \mathbf{1}_E}_{H_S} + \mathbf{1}_S \otimes \underbrace{\sum_k \omega_k a_k^\dagger a_k}_{H_E} + \lambda \underbrace{\sigma_1 \otimes B}_{H'} ; \quad (104)$$

here, $B = B^\dagger$ is any observable of E with $\text{Tr}[\rho_E B] = 0$, where, as in Example 3.3, the environment reference state is given by

$$\rho_E = \frac{e^{-\beta H_E}}{\text{Tr}[e^{-\beta H_E}]} . \quad (105)$$

Using the fact that

$$\sigma_1(s) = e^{is\Omega\sigma_3/2} \sigma_1 e^{-is\Omega\sigma_3/2} = \cos(s\Omega) \sigma_1 - \sin(s\Omega) \sigma_2 ,$$

the resulting master equation derived by means of the same Markov approximation used for (100) reads, with $G(s) \equiv \text{Tr}[\rho_E B(s) B]$,

$$\partial_t \rho_S(t) = i \frac{\Omega}{2} [\sigma_3, \rho_S(t)] + \lambda^2 \mathbb{D}_1[\rho_S(t)] , \quad (106)$$

where

$$\begin{aligned} \mathbb{D}_1[\rho_S(t)] = & \int_0^\infty ds \left\{ G(s) \left(\cos(s\Omega) [\sigma_1, \sigma_1 \rho_S(t)] - \sin(s\Omega) [\sigma_2, \sigma_1 \rho_S(t)] \right) \right. \\ & \left. + G(-s) \left(\cos(s\Omega) [\rho_S(t) \sigma_1, \sigma_1] - \sin(s\Omega) [\rho_S(t) \sigma_1, \sigma_2] \right) \right\} . \end{aligned} \quad (107)$$

In order to discuss the implication of this Markov approximation, it proves convenient to adopt the vector representation (52). Therefore, we insert the expansion of $\rho_S(t)$ along the Pauli matrices as in (51); this yields the following expression for the matrix \mathcal{H} and \mathcal{D} :

$$\mathcal{H} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \Omega/2 & 0 \\ 0 & -\Omega/2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} , \quad \mathcal{D}_1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & \alpha & 0 \\ d & 0 & 0 & \alpha \end{pmatrix} , \quad (108)$$

where

$$\begin{aligned}\alpha &= \lambda^2 \int_0^\infty ds \cos(s\Omega) (G(s) + G(-s)) \\ &= \frac{\lambda^2}{2} \int_{-\infty}^{+\infty} ds e^{i\Omega s} G(s) + \frac{\lambda^2}{2} \int_{-\infty}^{+\infty} ds e^{-i\Omega s} G(s) ,\end{aligned}\quad (109)$$

$$b = \lambda^2 \int_0^\infty ds \sin(s\Omega) (G(s) + G(-s)) , \quad (110)$$

$$\begin{aligned}d &= i \lambda^2 \int_0^\infty ds \sin(s\Omega) (G(s) - G(-s)) \\ &= \frac{\lambda^2}{2} \int_{-\infty}^{+\infty} ds e^{i\Omega s} G(s) - \frac{\lambda^2}{2} \int_{-\infty}^{+\infty} ds e^{-i\Omega s} G(s) .\end{aligned}\quad (111)$$

Because of b , the 3×3 matrix $\mathcal{D}_1^{(3)} = \begin{pmatrix} 0 & b & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{pmatrix}$ is not hermitian. However, it splits into a symmetric and anti-symmetric part:

$$\mathcal{D}_1 = \underbrace{\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & b/2 & 0 \\ 0 & -b/2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}}_{\mathcal{H}^{(2)}} + \underbrace{\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & b/2 & 0 \\ 0 & b/2 & \alpha & 0 \\ d & 0 & 0 & \alpha \end{pmatrix}}_{\mathcal{D}} ; \quad (112)$$

the contribution $\mathcal{H}^{(2)}$ can be absorbed into \mathcal{H} as a second order correction to the free Hamiltonian. Now the corresponding matrix $\mathcal{D}^{(3)}$ is hermitian, but, again because of b , apparently non-positive. Suppose $b = 0$, in order to check that the generated semigroup is positivity preserving, according to (59), it is necessary that $\alpha \geq 0$. This is indeed so: in fact, from the KMS conditions (103) applied to the thermal state ρ_E , it follows that

$$\alpha + d = \lambda^2 \int_{-\infty}^{+\infty} ds e^{is\Omega} G(s) , \quad \alpha - d = e^{-\beta\Omega}(\alpha + d) . \quad (113)$$

If we thus show that $\alpha + d \geq 0$, then $\alpha \geq 0$; this is achieved by explicitly computing the two-point correlation function within the simplifying framework where ρ_E is effectively a density matrix, with orthonormal basis $H_E|\varepsilon_j\rangle = \varepsilon_j|\varepsilon_j\rangle$. With \mathcal{Z}_β the normalization of ρ_E ,

$$\begin{aligned}\alpha + d &= \mathcal{Z}_\beta \int_{-\infty}^{+\infty} ds e^{is\Omega} \text{Tr} \left(e^{-\beta H_E} e^{is H_E} B e^{-is H_E} B \right) \\ &= \mathcal{Z}_\beta \sum_{j,k} e^{-\beta \varepsilon_j} |\langle \varepsilon_j | B | \varepsilon_k \rangle|^2 \int_{-\infty}^{+\infty} ds e^{is(\Omega + \varepsilon_j - \varepsilon_k)} \\ &= 2\pi \mathcal{Z}_\beta \sum_{j,k} e^{-\beta \varepsilon_j} |\langle \varepsilon_j | B | \varepsilon_k \rangle|^2 \delta(\Omega + \varepsilon_j - \varepsilon_k) \geq 0 .\end{aligned}\quad (114)$$

We are now in position to study the consequences of the presence of b and d . We shall use the same argument developed in Example 3.1; at time $t = 0$, (55) gives

$$\frac{d}{dt}\text{Det}(\rho) = 2b\rho_1\rho_2 + \alpha\rho_2^2 + d\rho_3 + \alpha\rho_3^2 .$$

One checks that

$$\rho_1 = \frac{1}{2}\sqrt{\frac{4\alpha^2 - d^2}{\alpha^2 + b^2}} , \quad \rho_2 = -\frac{b}{2\alpha}\sqrt{\frac{4\alpha^2 - d^2}{\alpha^2 + b^2}} , \quad \rho_3 = -\frac{d}{2\alpha} ,$$

fulfil $\rho_1^2 + \rho_2^2 + \rho_3^2 = 1$ and thus give a pure state $\rho = P$ ($\text{Det}(P) = 0$). Moreover, unless $b = d = 0$,

$$\frac{d}{dt}\text{Det}(P) = -\frac{\alpha(4b^2 + d^2)}{4(\alpha^2 + b^2)} < 0 .$$

Because of (103), even if $b = 0$, $d = 0$ is possible only at infinite temperature, that is when $\beta = 0$. It thus follows, that at finite temperature, the Markov approximation discussed in this Section does not preserve positivity, since a state like P is immediately turned into an operator with negative determinant, thus signalling the emergence of negative eigenvalues in its spectrum.

Despite this physical inconsistency, the semigroup γ_t generated by $\mathcal{H} + \mathcal{D}$ in (108) is nevertheless often used in phenomenological applications on the basis of its good asymptotic behaviour. In fact, it has a unique equilibrium state ρ_{eq} which is easily obtained from the condition $(\mathcal{H} + \mathcal{D})|\rho_{eq}\rangle = 0$, yielding $\rho_1 = \rho_2 = 0$ and $\rho_3 = -d/\alpha$. Using (113), this gives:

$$\rho_{eq} = \frac{1}{e^{\beta\Omega/2} + e^{-\beta\Omega/2}} \begin{pmatrix} e^{-\beta\Omega/2} & 0 \\ 0 & e^{\beta\Omega/2} \end{pmatrix} = \frac{e^{-\beta H_S}}{\text{Tr}[e^{-\beta H_S}]} . \quad (115)$$

Therefore, as expected, the bath drives the embedded open system at equilibrium at its own temperature. Nevertheless, as we shall see next, there is no need to use an unphysical treatment in order to get a Markovian evolution leading to asymptotic relaxation to equilibrium. \square

Remark 3.6 The origin of the lack of positivity-preservation lies in the way the free time-evolution generated by H_S interferes with the various truncations. Indeed, if $\Omega = 0$, so that there is no free evolution of S , then $d = b = 0$. Observe, however, that in this case, according to (58), the dynamical maps γ_t turn out to be completely positive and not only positive. In the next Section, we shall see a particular way to deal with the free evolution that automatically leads to a semigroup of completely positive maps. \square

3.3.2. Weak Coupling Limit

In order to obtain a physically consistent Markovian approximation of (92) in the limit of weak couplings, a more careful derivation is needed.⁷¹ The formal integration

of equation (96),

$$\rho_S(t) = e^{t\mathbb{L}_S^\lambda}[\rho_S(0)] + \lambda^2 \int_0^t ds e^{(t-s)\mathbb{L}_S^\lambda} \circ \mathbb{D}_1[\rho_S(s)] , \quad (116)$$

can be rewritten as

$$e^{-t\mathbb{L}_S^\lambda} \rho_S(t) = \rho_S(0) + \lambda^2 \int_0^t ds \left(e^{-s\mathbb{L}_S^\lambda} \circ \mathbb{D}_1 \circ e^{s\mathbb{L}_S^\lambda} \right) \circ e^{-s\mathbb{L}_S^\lambda}[\rho_S(s)] . \quad (117)$$

Upon passing to the slow time $\tau = \lambda^2 t$, it reads

$$\begin{aligned} e^{-(\tau/\lambda^2)\mathbb{L}_S^\lambda} \rho_S(\tau/\lambda^2) &= \rho_S(0) \\ &+ \int_0^\tau ds \left(e^{-(s/\lambda^2)\mathbb{L}_S^\lambda} \circ \mathbb{D}_1 \circ e^{(s/\lambda^2)\mathbb{L}_S^\lambda} \right) \circ e^{-(s/\lambda^2)\mathbb{L}_S^\lambda}[\rho_S(s/\lambda^2)] . \end{aligned} \quad (118)$$

Using (98) and (100) one has

$$\begin{aligned} e^{-(s/\lambda^2)\mathbb{L}_S^\lambda} \circ \mathbb{D}_1 \circ e^{(s/\lambda^2)\mathbb{L}_S^\lambda}[\rho_S] &= - \sum_{\alpha,\beta} \int_0^\infty du \\ &\times \left\{ G_{\alpha\beta}(u) \left[e^{(is/\lambda^2)H_S^\lambda} V_\alpha(u) e^{-(is/\lambda^2)H_S^\lambda} , e^{(is/\lambda^2)H_S^\lambda} V_\beta e^{-(is/\lambda^2)H_S^\lambda} \rho_S \right] \right. \\ &\left. + G_{\beta\alpha}(-u) \left[\rho_S e^{(is/\lambda^2)H_S^\lambda} V_\beta e^{-(is/\lambda^2)H_S^\lambda} , e^{(is/\lambda^2)H_S^\lambda} V_\alpha(u) e^{-(is/\lambda^2)H_S^\lambda} \right] \right\} . \end{aligned} \quad (119)$$

For sake of simplicity, we assume now the effective Hamiltonian H_S^λ to have discrete spectrum $H_S^\lambda = \sum_{a=1}^n \varepsilon_a^\lambda P_a^\lambda$. By inserting $\sum_{a=1}^n P_a^\lambda = \mathbf{1}_n$ into (119), we get

$$\begin{aligned} e^{-(s/\lambda^2)\mathbb{L}_S^\lambda} \circ \mathbb{D}_1 \circ e^{(s/\lambda^2)\mathbb{L}_S^\lambda}[\rho_S] &= - \sum_{\alpha,\beta} \sum_{a,b,c,d=1}^n \int_0^\infty du e^{is[\varepsilon_a^\lambda - \varepsilon_b^\lambda - (\varepsilon_d^\lambda - \varepsilon_c^\lambda)]/\lambda^2} \times \\ &\times \left\{ G_{\alpha\beta}(u) \left[P_a^\lambda V_\alpha(u) P_b^\lambda , P_c^\lambda V_\beta P_d^\lambda \rho_S \right] \right. \\ &\left. + G_{\beta\alpha}(-u) \left[\rho_S P_a^\lambda V_\beta P_b^\lambda , P_c^\lambda V_\alpha(u) P_d^\lambda \right] \right\} . \end{aligned} \quad (120)$$

When $\lambda \rightarrow 0$, only the exponentials with $\varepsilon_a^\lambda - \varepsilon_b^\lambda = \varepsilon_d^\lambda - \varepsilon_c^\lambda$ are expected to effectively contribute, since otherwise the term within parenthesis in (118) rapidly oscillates, giving vanishingly small contributions; this approximation is known as *rotating-wave approximation*. Also, under suitable assumptions, when $\lambda \rightarrow 0$, the eigenvalues ε_a^λ and the eigenprojections P_a^λ are expected to go into eigenvalues ε_a and eigenprojectors P_a of H_S .

In more mathematically precise terms, one can show that the oscillating term can be substituted by the following ergodic average:^{72,73}

$$\tilde{\mathbb{D}} \equiv \lim_{T \rightarrow +\infty} \frac{1}{2T} \int_{-T}^{+T} ds e^{-s\mathbb{L}_{H_S}} \circ \mathbb{D}_1 \circ e^{s\mathbb{L}_S} . \quad (121)$$

Further, when $\lambda \rightarrow 0$, $\tilde{\mathbb{D}}$ commutes with $e^{-(s/\lambda^2)\mathbb{L}_S^\lambda}$, so that, one finally gets the Markov approximation

$$\rho_S(t) = e^{t\mathbb{L}_S^\lambda}[\rho_S(0)] + \lambda^2 \int_0^t ds e^{(t-s)\mathbb{L}_S^\lambda} \circ \tilde{\mathbb{D}}[\rho_S(s)] , \quad (122)$$

which solves the master equation

$$\partial_t \rho_S(t) = \mathbb{L}_S^\lambda[\rho_S(t)] + \lambda^2 \tilde{\mathbb{D}}[\rho_S(t)] . \quad (123)$$

Before discussing in details the form of the dissipative term $\tilde{\mathbb{D}}$, we reconsider Example 3.4.

Example 3.5 In the vectorial representation of Example 3.1, the free time-evolution amounts to the 4×4 matrix

$$\mathcal{U}_s^S = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(s\Omega) & -\sin(s\Omega) & 0 \\ 0 & \sin(s\Omega) & \cos(s\Omega) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} ,$$

which yields the ergodic average

$$\lim_{T \rightarrow +\infty} \frac{1}{2T} \int_{-T}^{+T} ds \left(\mathcal{U}_s^S \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & \alpha & 0 \\ d & 0 & 0 & \alpha \end{pmatrix} \mathcal{U}_{-s}^S \right) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \alpha/2 & b/2 & 0 \\ 0 & -b/2 & \alpha/2 & 0 \\ d & 0 & 0 & \alpha \end{pmatrix} . \quad (124)$$

From the averaged matrix we extract the antisymmetric part

$$\mathcal{H}^{(2)} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & b/2 & 0 \\ 0 & -b/2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} , \quad (125)$$

which gives a second order correction to \mathcal{H} in (109), and the dissipative term

$$\mathcal{D}_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \alpha/2 & 0 & 0 \\ 0 & 0 & \alpha/2 & 0 \\ d & 0 & 0 & \alpha \end{pmatrix} . \quad (126)$$

A part from the entry d , we see that the 3×3 matrix $\mathcal{D}_2^{(3)}$ satisfies the conditions (58); also, the presence of d does not spoil the complete positivity of the generated map γ_t , for, as we shall show, the ergodic average automatically yields completely positive semigroups. We conclude the example by noticing that the equilibrium state, determined by $(\mathcal{H} + \mathcal{H}^{(2)} + \mathcal{D}_2)|\rho_{eq}\rangle = 0$ is as in (115). \square

In order to prove the claim at the end of the preceding Example, we now study in detail the structure of (121) and show that it amounts to a generator as in (47)–(48) with positive Kossakowski matrix.

We set $\omega = \varepsilon_a - \varepsilon_b$ with ε_a running over the spectrum of H_S ; by means of the decompositions

$$V_\alpha(\omega) \equiv \sum_{\varepsilon_a - \varepsilon_b = \omega} P_a V_\alpha P_b, \quad V_\beta(-\omega) \equiv \sum_{\varepsilon_d - \varepsilon_c = \omega} P_c V_\beta P_d = V_\beta^\dagger(\omega), \quad (127)$$

from (120) and (121), we explicitly get

$$\begin{aligned} \tilde{\mathbb{D}}[\rho_S] = & - \sum_{\alpha, \beta} \sum_{\omega} \int_0^\infty du \left\{ e^{iu\omega} G_{\alpha\beta}(u) \left[V_\alpha(\omega), V_\beta^\dagger(\omega) \rho_S \right] \right. \\ & \left. + e^{-iu\omega} G_{\beta\alpha}(-u) \left[\rho_S V_\beta(\omega), V_\alpha^\dagger(\omega) \right] \right\}. \quad (128) \end{aligned}$$

Further, it follows from standard Fourier analysis that¹

$$\int_0^\infty dt e^{it\omega} G_{\alpha\beta}(t) = \frac{h_{\alpha\beta}(\omega)}{2} + i s_{\alpha\beta}(\omega), \quad (129)$$

where

$$h_{\alpha\beta}(\omega) \equiv \int_{-\infty}^{+\infty} dt e^{it\omega} G_{\alpha\beta}(t) = h_{\beta\alpha}^*(\omega) \quad (130)$$

is a positive matrix,ⁱ while

$$s_{\alpha\beta}(\omega) \equiv \frac{1}{2\pi} \mathcal{P} \int_{-\infty}^{+\infty} dw \frac{h_{\alpha\beta}(\omega)}{w - \omega} = s_{\beta\alpha}^*(\omega), \quad (131)$$

and \mathcal{P} indicates principal value. In terms of the Fourier transforms of the two-point correlation functions of the environment, one then rewrites

$$\tilde{\mathbb{D}}[\rho_S] = -i \underbrace{\left[\sum_{\alpha, \beta} \sum_{\omega} s_{\alpha\beta}(\omega) V_\alpha(\omega) V_\beta^\dagger(\omega), \rho_S \right]}_{H_E^{(2)}} \quad (132)$$

$$+ \underbrace{\sum_{\alpha, \beta} \sum_{\omega} h_{\alpha\beta}(\omega) \left(V_\beta^\dagger(\omega) \rho_S V_\alpha(\omega) - \frac{1}{2} \left\{ V_\alpha(\omega) V_\beta^\dagger(\omega), \rho_S \right\} \right)}_{\mathbb{D}_2}. \quad (133)$$

We thus arrive at the following explicit form of the generator (123)

$$\partial_t \rho_S(t) = -i \left[H_S + \lambda H_E^{(1)} + \lambda^2 H_E^{(2)}, \rho_S(t) \right] + \lambda^2 \mathbb{D}_2[\rho_S(t)]. \quad (134)$$

We thus see that, beside the second order dissipative term of the form (49), the environment contributes with a first-order mean-field term and also a second order

ⁱThis can be proved by applying to $h_{\alpha\beta}(\omega)$ considerations similar to the ones employed in (114) of Example 3.4 that use the spectral decomposition of the environment time-evolution.

term to the redefinition of an effective Hamiltonian of S . Further, the Kossakowski matrices $[h_{\alpha\beta}(\omega)]$ are positive-definite for all ω .

Remarks 3.7

- (1) Formally, the last statement above follows from Bochner's theorem (see for instance Appendix A.3 in Ref.[1]) which states that the Fourier transform $h_{\alpha\beta}(\omega)$ of a function of positive type, as the two-point correlation functions $G_{\alpha\beta}(t)$, gives rise to a positive-definite matrix.
- (2) The ergodic average elimination of the rapid oscillations due to the free system dynamics results in a semigroup consisting of completely positive maps.
- (3) An equivalent derivation of the physically consistent Markovian master equation (134) can be obtained through the so-called *stochastic limit*:^{74,75} it provides a different, more abstract justification for the ergodic average (121).
- (4) A so-called quantum FokkerPlanck master equation has been derived in [76]; it provides a description of quantum Brownian motion with additional corrections due to quantum statistics. \square

The mathematical consistency of the previous manipulations rests on some assumptions on the behaviour of two-point correlation functions. In particular, as proven in Refs.[72, 73], the following conditions turn out to be sufficient. The first one is a condition on the norms of the system observables V_α which are coupled to the environment, that is $\sum_\alpha \|V_\alpha\| < \infty$. The second is an assumption on the environment which is assumed to be *quasi-free*, namely all its higher time-correlation functions can be expressed as sums of two-point correlation functions. The third regards the decay of two-point correlation functions which is assumed to be such that there exists $\eta > 0$ for which

$$\int_0^\infty dt |G_{\alpha\beta}(t)| (1+t)^\eta < a, \quad (135)$$

with a independent of α, β .

Remark 3.8 The derivation of the master equation (134) is based on the assumption of a weak coupling between subsystem and external bath; a master equation of the same kind can also describe a different situation, in which the interactions between subsystem and environment are rare, but not necessarily weak. The typical instance is that of an atom, effectively modeled as an n -level system, immersed in a rarefied gas, that represents the environment. The collisions of the atom with the gas particles are described by the scattering operator, which involves the full interaction Hamiltonian; however, these are rare events, since the gas is by hypothesis very dilute. Using mathematically rigorous techniques, one can then show that in the so-called *low density limit* the atom subdynamics is generated by a master equation in Kossakowski-Lindblad form.^{77,1,5} \square

3.3.3. Singular Coupling Limit

Unlike in the weak coupling limit, in the singular coupling regime, it is the decay time of correlations in the environment that becomes small, $\tau_E \rightarrow 0$, while the typical variation time of ρ_S , τ_S , stays constant. Concretely, the two-point correlation functions appearing in the dissipative contributions to the open dynamics are made tend to Dirac deltas:^{54,78,79}

$$G_{\alpha\beta}(t) \rightarrow C_{\alpha\beta} \delta(t) , \quad (136)$$

so that the dissipative effects manifest themselves on time-scales of order t .

In order to implement such a behaviour and derive the corresponding master equation, we consider (17) and rescale it as follows:³

$$H_{S+E} = H_S \otimes \mathbf{1}_E + \varepsilon^{-2} \mathbf{1}_S \otimes H_E + \varepsilon^{-1} H' . \quad (137)$$

Here we assume $H' = \sum_{\alpha} V_{\alpha} \otimes B_{\alpha}$, with centered environment operators B_{α} , *i.e.* $\text{Tr}[B_{\alpha} \rho_E] = 0$. Then, the same steps leading to (93) yield

$$\begin{aligned} \rho_S(t) = e^{t\mathbb{L}_{H_S}}[\rho_S(0)] - \varepsilon^{-2} \int_0^t dv \int_0^v du e^{(t-v)\mathbb{L}_S} \times \\ \times \text{Tr}_E \left(\left[H' , e^{u\mathbb{L}^{Q,Q}} \left[H' , \rho_S(v-u) \otimes \rho_E \right] \right] \right) . \end{aligned} \quad (138)$$

By letting $u = \varepsilon^2 w$ and $\varepsilon \rightarrow 0$, one formally gets

$$\begin{aligned} \rho_S(t) = e^{t\mathbb{L}_{H_S}}[\rho_S(0)] - \int_0^t dv e^{(t-v)\mathbb{L}_{H_S}} \times \\ \times \int_0^\infty du \text{Tr}_E \left(\left[H' , e^{u\mathbb{L}_{H_E}} \left[H' , \rho_S(v) \otimes \rho_E \right] \right] \right) . \end{aligned} \quad (139)$$

Explicitly, the above expression solves the evolution equation

$$\partial_t \rho_S(t) = -i \left[H_S , \rho_S(t) \right] + \hat{\mathbb{D}}[\rho_S(t)] , \quad (140)$$

where

$$\begin{aligned} \hat{\mathbb{D}}[\rho_S(t)] = - \sum_{\alpha,\beta} \int_0^\infty ds \left\{ G_{\alpha\beta}(s) \left[V_{\alpha} , V_{\beta} \rho_S(t) \right] \right. \\ \left. + G_{\beta\alpha}(-s) \left[\rho_S(t) V_{\beta} , V_{\alpha} \right] \right\} . \end{aligned} \quad (141)$$

As was done in the weak coupling regime, one writes

$$\int_0^\infty G_{\alpha\beta}(s) ds = \frac{h_{\alpha\beta}}{2} + i s_{\alpha\beta} ,$$

so that (141) splits into a second-order Hamiltonian contribution, with Hamiltonian

$$H^{(2)} = \sum_{\alpha,\beta} s_{\alpha\beta} V_{\alpha} V_{\beta} , \quad (142)$$

and a true dissipative term of the form:

$$\mathbb{D}_3[\rho_S] = \sum_{\alpha, \beta} h_{\alpha\beta} \left(V_\beta \rho_S V_\alpha - \frac{1}{2} \{ V_\alpha V_\beta, \rho_S \} \right). \quad (143)$$

Altogether, this yields the following semigroup generator:

$$\partial_t \rho_S(t) = -i \left[H_S + H_E^{(2)}, \rho_S(t) \right] + \mathbb{D}_3[\rho_S(t)]. \quad (144)$$

Remarks 3.9

- (1) The singular coupling limit, as well as the weak coupling limit, leads to a generator of the Lindblad form (49) with a positive Kossakowski matrix and thus to a dissipative semigroup consisting of completely positive maps. Notice that, unlike in the weak coupling limit case, the operators contributing to the dissipative term \mathbb{D}_3 are hermitian.
- (2) By going to the slow time $\tau = \varepsilon^2 t$, the global Hamiltonian (137) becomes

$$H_{S+E} = \varepsilon^2 H_S \otimes \mathbf{1}_E + \mathbf{1}_S \otimes H_E + \varepsilon H'. \quad (145)$$

This shows that the singular coupling limit amounts to a weak coupling limit where the free motion generated by the Hamiltonian H_S is of the same order of the dissipative effects.^{80,3}

- (3) Unlike the weak coupling limit, thermal Bose or Fermi heat baths provide frameworks suited to the singular coupling limit only if their temperature is infinite.^{2,78,79} Indeed, the two-point correlation functions may tend to Dirac deltas in time only if their Fourier transforms tend to a constant, but this is in contradiction with the KMS-conditions (103), unless $\beta = 0$ and thus $T = \infty$.
- (4) The infinite temperature limit is equivalent to add to the system Hamiltonian H_S an external Gaussian stochastic potential $V(t)$.^j In such a case, the partial trace Tr_E with respect to ρ_E , is substituted by the average with respect to the Gaussian noise driving $V(t)$.⁷⁸ The resulting generator is as in (144) with a real-symmetric Kossakowski matrix $[h_{\alpha\beta}]$ (for a specific instance, see Example 3.8 below); consequently, the totally depolarized state $\tau_n = \mathbf{1}_n/n$ is an invariant equilibrium state and corresponds to the state (115) with $\beta = 0$, that is at infinite temperature. \square

Example 3.6 We now reexamine Example 3.4 in the light of the singular coupling limit; thus, we consider the rescaled total Hamiltonian

$$H_{S+E} = \frac{\Omega}{2} \sigma_3 \otimes \mathbf{1}_E + \mathbf{1}_S \otimes \varepsilon^{-2} \sum_k \omega_k a_k^\dagger a_k + \varepsilon^{-1} \sigma_1 \otimes B, \quad (146)$$

^jThis approximation is very useful in many phenomenological applications, in particular for treating decoherence effects in the propagation of elementary particles in matter; for details, see Refs.[81, 82].

With respect to (108) and (126), in the vectorial representation, the singular coupling limit gives the following dissipative matrix

$$\mathcal{D}_3 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \alpha & 0 \\ 0 & 0 & 0 & \alpha \end{pmatrix}, \quad \text{where now} \quad \alpha = 2 \operatorname{Re} \left(\int_0^\infty dt G(t) \right). \quad (147)$$

This result directly follows from (109)–(111) by setting $\Omega = 0$ and thus neglecting the free system time-evolution whence $b = d = 0$. By the same argument developed in Example 3.4, it turns out that $\alpha \geq 0$ and the generated semigroup consists of completely positive maps. \square

3.3.4. A Convolution-Free Master Equation

The Markov approximations presented in the previous three sections all start from the convolution master equation (80). There is however a derivation which is convolution-free and also leads to the Redfield-type equations as in (96).⁶⁰

Within the approximation of weak coupling between system and environment ($\lambda \ll 1$), one starts from the complete master equation for the compound system $T = S + E$,

$$\partial_t \rho_T(t) = (\mathbb{L}_0 + \lambda \mathbb{L}')[\rho_T(t)],$$

where \mathbb{L}_0 comprises commutators with respect to system and environment Hamiltonians and \mathbb{L}' the commutator with an interaction Hamiltonian as in (74), with centered environment observables. One then passes to the interaction representation $\tilde{\rho}_T(t) \equiv \exp(-t\mathbb{L}_0)[\rho_T(t)]$ and solves iteratively the resulting time-dependent evolution equation

$$\partial_t \tilde{\rho}_T(t) = \lambda \mathbb{L}'(t)[\tilde{\rho}_T(t)], \quad \mathbb{L}'(t) \equiv e^{-t\mathbb{L}_0} \mathbb{L}' e^{t\mathbb{L}_0}.$$

With initial condition $\tilde{\rho}_T(0) = \rho_T(0)$, the solution can be expressed as a series expansion in the small parameter λ :

$$\tilde{\rho}_T(t) = \sum_{k=0}^{\infty} \lambda^k \mathbb{N}_k(t)[\tilde{\rho}_T(0)],$$

where

$$\mathbb{N}_k(t)[\tilde{\rho}_T(0)] \equiv \int_0^t ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{k-1}} ds_k \mathbb{L}'(s_1) \circ \mathbb{L}'(s_2) \cdots \circ \mathbb{L}'(s_k)[\rho_T(0)],$$

and $\mathbb{N}_0(t)[\rho_T(0)] \equiv \rho_T(0)$.

Under the hypothesis of a factorized initial state, $\rho_T(0) = \rho_S \otimes \rho_E$, with ρ_E an environment equilibrium state, $\mathbb{L}_{H_E}[\rho_E] = 0$, using the projection introduced in (66), one gets

$$P[\tilde{\rho}_T(t)] = \underbrace{\operatorname{Tr}_E[\tilde{\rho}_T(t)]}_{\tilde{\rho}_S(t)} \otimes \rho_E = \sum_{k=0}^{\infty} \lambda^k \operatorname{Tr}_E \left(\mathbb{N}_k(t)[\rho_S \otimes \rho_E] \right) \otimes \rho_E.$$

Further, setting

$$\mathcal{M}_k(t)[\rho_S] \equiv \text{Tr}_E \left(\mathbb{N}_k(t)[\rho_S \otimes \rho_E] \right), \quad \Phi_t \equiv \sum_{k=0}^{\infty} \lambda^k \mathcal{M}_k(t), \quad (148)$$

one writes $\tilde{\rho}_S(t) = \Phi_t[\rho_S(0)]$ and, by a formal inversion of Φ_t , one gets

$$\partial_t \tilde{\rho}_S(t) = \dot{\Phi}_t[\rho_S(0)] = \dot{\Phi}_t \circ \Phi_t^{-1}[\tilde{\rho}_S(t)].$$

Due to the Tr_E operation, the operators $\mathcal{M}_k(t)$ contain k -time correlation functions of the environment. At this point one makes the assumption of a thermal environment for which only even correlation functions matter and, according to the weak coupling assumption, expand to lowest order in λ^2 , $\dot{\Phi}_t \circ \Phi_t^{-1} \simeq \lambda^2 \dot{\mathcal{M}}_2(t)$. Returning to the Schrödinger picture and explicitly inserting the environment two-point correlation functions one gets the Redfield-type equations

$$\partial_t \rho_S(t) = -i[H_S, \rho_S(t)] + \mathbb{D}_4[\rho_S(t)], \quad (149)$$

where

$$\begin{aligned} \mathbb{D}_4[\rho_S(t)] = \sum_{\alpha\beta} \int_0^\infty ds \Big\{ & G_{\alpha\beta}(s) [V_\beta(-s) \rho_S(t), V_\alpha] \\ & + G_{\beta\alpha}(-s) [V_\alpha, \rho_S(t) V_\beta(-s)] \Big\}. \end{aligned} \quad (150)$$

The dissipative term \mathbb{D}_4 in the above time-evolution equation is rather similar to (100) and thus suffers from the same problems in relations to positivity-preservation. This is explicitly shown by the following example.

Example 3.7 Let us consider Example 3.4 in the light of the convolutionless approach; in the vectorial representation, it gives the following dissipative matrix

$$\tilde{\mathcal{D}}_4 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & -b & \alpha & 0 \\ d & 0 & 0 & \alpha \end{pmatrix}, \quad (151)$$

where α , b and d are as in Example 3.4. As done there, we split the 3×3 matrix $\tilde{\mathcal{D}}_4^{(3)} = \begin{pmatrix} 0 & 0 & 0 \\ -b & \alpha & 0 \\ 0 & 0 & \alpha \end{pmatrix}$ into symmetric and anti-symmetric part. The first term provides a second order correction $\mathcal{H}^{(2)}$ to the free-Hamiltonian term, while the second one gives rise to a dissipative term

$$\mathcal{D}_4 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -b/2 & 0 \\ 0 & -b/2 & \alpha & 0 \\ d & 0 & 0 & \alpha \end{pmatrix},$$

of the same form as \mathcal{D}_1 in Example 3.4, see the second piece in (112), with $b \rightarrow -b$. Therefore, unless $b = d = 0$, there exist initial states that, as four-dimensional vectors, are mapped by the semigroup

$$\mathcal{G}_t = \exp\left[t(\mathcal{H} + \mathcal{H}^{(2)} + \mathcal{D}_4)\right]$$

into vectors, corresponding to matrices with negative eigenvalues. \square

Further elaborations are then needed to make physically acceptable the dynamics obtained by the convolutionless method.

Remark 3.10 A cure against lack of complete positivity and even of positivity has been put forward which is based on the so-called *slippage of initial conditions* (see, Refs.[63-66]). The argument is that any Markov approximation neglects a certain initial span of time, namely a transient, during which no semigroup time-evolution is possible due to unavoidable memory effects. The transient dynamics can be effectively depicted as a slippage operator that, out of all possible initial states, selects those which can not conflict with the Markov time-evolution when it sets in. As we shall see in the next Section, the slippage-argument may cure the positivity-preserving problem, but misses the point about the complete positivity issue which emerges in full only when dealing with bi- and multi-partite open quantum systems and with the existence of entangled states.⁸³ \square

The convolutionless approach is often advocated in situations where, instead of a weak coupling to an environment, the open system is affected by a weak stochastic potential.^{60,61,62} As already observed in Remark 3.9.4, one substitutes the trace with respect to the environment degrees of freedom by an average over the noise. Experimental contexts where one can simulate external noisy potentials seem to be feasible; by modulating the noise one can enhance the non-positivity preserving character of the Redfield-type equations and thus expose the physical inconsistency of the Markovian approximation on which they are based.^{23,26,32}

In particular, neutron interferometry, which has proved to be an extremely powerful tool to investigate gravitational, inertial and phase-shifting effects occurring inside the interferometer,^k may be used to investigate the notion of completely positive open system dynamics. In order to do that, we consider below the case in which neutrons while propagating inside the interferometric apparatus are subjected to weak time-dependent, stochastic magnetic fields coupled to their spin degree of freedom. In this case, the noisy effects result from the classical stochastic character of the fields and not from an interaction with a quantum environment.

^kFor an account of relevant results, see *e.g.* Refs.[84, 85].

Example 3.8 The states of the neutrons inside the interferometer can then be described by a 2×2 density matrix $R(t)$. Its dynamics is generated by a time-dependent Hamiltonian that takes the form

$$H(t) = \frac{\Omega}{2} \sigma_3 + \vec{\sigma} \cdot \vec{\mathbf{B}}(t) , \quad (152)$$

where the system Hamiltonian H_S is as in Example 3.3, while $\mathbf{B}(t) = (B_1(t), B_2(t), B_3(t))$ represents a Gaussian stochastic magnetic field. We assume $\mathbf{B}(t)$ to have zero mean, $\langle \mathbf{B}(t) \rangle = 0$, and a stationary, real, positive-definite covariance matrix $G_{ij}(t)$ with entries

$$G_{ij}(t-s) = \langle B_i(t) B_j(s) \rangle = G_{ij}^*(t-s) = G_{ji}(s-t) . \quad (153)$$

The time-dependent evolution equation for the density matrix R describing the spin degree of freedom splits into

$$\partial_t R(t) = (\mathbb{L}_0 + \mathbb{L}_t)[R(t)] , \quad (154)$$

$$\mathbb{L}_0[R(t)] = -i \left[\frac{\Omega}{2} \sigma_3 , R(t) \right] , \quad \mathbb{L}_t[R(t)] = -i \left[\mathbf{B}(t) \cdot \vec{\sigma} , R(t) \right] . \quad (155)$$

Because of the stochastic field $\vec{\mathbf{B}}(t)$, the solution $R(t)$ of (154) is also stochastic; an effective spin density matrix $\rho(t) \equiv \langle R(t) \rangle$ is obtained by averaging over the noise. At time $t = 0$ we may suppose spin and noise to decouple so that the initial state is $\rho \equiv \langle R(0) \rangle = R(0)$.

The effective time-evolution of $\rho(t)$ can naturally be obtained following the techniques of the previous Section, where the trace over the environment degrees of freedom is substituted by the average over the classical noise, $\text{Tr}_E \rightarrow \langle \cdot \rangle$. The resulting master equation has the form (150):

$$\partial_t \rho_S(t) = -i \left[\frac{\Omega}{2} \sigma_3 , \rho(t) \right] + \tilde{\mathbb{D}}_4[\rho(t)] , \quad (156)$$

where

$$\tilde{\mathbb{D}}_4[\rho(t)] = - \sum_{i,j} \int_0^\infty ds \, G_{ij}(s) \left[\sigma_i , \left[\sigma_j(-s) , \rho(t) \right] \right] . \quad (157)$$

The time dependent $\sigma_j(-s)$ explicitly reads:

$$\sigma_j(s) = e^{isH_S} \sigma_j e^{-isH_S} \equiv \sum_{k=1}^3 U_{jk}(s) \sigma_k ,$$

where

$$U_{jk}(s) = \begin{pmatrix} \cos \Omega s & -\sin \Omega s & 0 \\ \sin \Omega s & \cos \Omega s & 0 \\ 0 & 0 & 1 \end{pmatrix} .$$

Inserting these expressions in (157), and extracting the symmetric and antisymmetric contributions, the master equation results of the form:

$$\partial_t \rho(t) = -i \left[H_S + H^{(2)} , \rho(t) \right] + \mathbb{D}_4[\rho(t)] , \quad (158)$$

where $H^{(2)} = \sum_{i,j,k=1}^3 \epsilon_{ijk} \kappa_{ij} \sigma_k$, and \mathbb{D}_4 is as in (50), with

$$\kappa_{ij} = \frac{1}{2} \sum_{k=1}^3 \int_0^\infty ds \left[G_{ik}(s) U_{kj}(-s) - U_{ik}(s) G_{kj}(-s) \right], \quad (159)$$

$$C_{ij} = \sum_{k=1}^3 \int_0^\infty ds \left[G_{ik}(s) U_{kj}(-s) + U_{ik}(s) G_{kj}(-s) \right]. \quad (160)$$

We now study the positivity and complete positivity of the generated time-evolution in relation to the decay properties of the stochastic magnetic field correlation matrix $G_{ij}(t)$. We will consider two representative cases.

- *White Noise*

Let the stochastic magnetic field have white-noise correlations $G_{ij}(t-s) = G_{ij} \delta(t-s)$, where the matrix G_{ij} is time-independent, symmetric and by assumption positive-definite. Hence, $\kappa_{ij} = 0$, and $C_{ij} = G_{ij}$, so that the Kossakowski matrix results positive definite and the generated semigroup is completely positive. Further, note that, due to the delta-correlations, all terms $\mathcal{M}_k(t)$, $k \geq 3$, in the expansion (148) identically vanish, so that the evolution equation (158) is in this case exact.⁷⁸

- *Single Component Covariance Matrix*

Consider a stochastic magnetic field along the x -direction, $\vec{B}(t) = (B(t), 0, 0)$, with

$$\langle B(t)B(s) \rangle = B^2 e^{-\lambda|t-s|}.$$

Then,

$$h_{ij} = \frac{\Omega B^2}{2(\lambda^2 + \Omega^2)} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad C_{ij} = \frac{B^2}{\lambda^2 + \Omega^2} \begin{pmatrix} 2\lambda & \Omega & 0 \\ \Omega & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Unless $\Omega = 0$ the matrix C_{ij} is not positive definite, and therefore the generated semigroup is surely not completely positive. Actually, adopting the vectorial formulation of Example 3.1 and setting:

$$\alpha = \frac{2B^2\lambda}{\lambda^2 + \Omega^2}, \quad b = \frac{B^2\Omega}{\lambda^2 + \Omega^2},$$

the relevant 3×3 dissipative matrix (56) reads

$$\mathcal{D}^{(3)} = \begin{pmatrix} 0 & -b & 0 \\ -b & \alpha & 0 \\ 0 & 0 & \alpha \end{pmatrix},$$

which is of the form of the previous Example 3.7; hence, even positivity is not preserved.

Although apparently formal, these results are not purely academic: indeed, the entries of $\rho(t)$ are directly accessible to experiments, where, by modulating a background magnetic field, one may get close to the stochastic properties of the two situations just analyzed. \square

3.4. *Why Completely Positive Semigroups?*

In the previous sections we have analyzed three Markov approximations that lead to reduced dynamics consisting of semigroups of trace and hermiticity preserving linear maps γ_t , $t \geq 0$, acting on the state-space of an open n -level system S . As emphasized before, any mathematical effective description of actual dissipative dynamics must in the first place preserve the positivity of any initial density matrix. Only in this case, the time-evolution turns out to be consistent with the interpretation of the state-eigenvalues as probabilities.

In the second place, one has also to care of possible couplings with inert and remote ancillas A and therefore to guarantee the positivity-preserving character of the semigroup of maps $\gamma_t \otimes \text{id}_A$, too; this is only assured if γ_t is completely positive.

The weak coupling limit with the ergodic average prescription and the singular coupling limit give semigroups of completely positive maps and therefore fully physically consistent. On the other hand, without ergodic average or through the convolutionless procedure one is led to Redfield-type equations which generate dynamical maps that are, in general, not even positivity preserving.

Remark 3.11 One can always construct semigroups of linear maps that are only positive and not completely positive, as seen in Example 3.1 (*cf.* Eq. (59)). The real problem is the derivation of such kind of dissipative dynamics from a microscopic interaction with the environment. One knows that these semigroups would not be acceptable in the case of couplings with ancillas: it is this inconsistency that essentially forbids their construction from microscopic interactions.^{72,71} Indeed, all known rigorous microscopic derivations of an open quantum reduced dynamics lead to completely positive semigroups. \square

It has also been remarked that complete positivity guarantees full physical consistency at the price of an order relation among typical life-times, which, in the two dimensional case is expressed by the necessary inequalities (58) (see also Example 3.2). It has been observed that from a strictly physical point of view, it appears doubtful that possible couplings to remote and inert ancillas might have concrete consequences on actual experimental contexts. In view of this, complete positivity is often refused as a mathematical artifact, with nice structural consequences as the Kossakowski-Lindblad form of the generators in (49), but without solid physical justifications.

Leaving aside the difficulty of deriving a positivity-preserving semigroup from fundamental system-environment interactions, one may argue that positivity preservation might suffice to guarantee physical consistency. Indeed, it is enough to ensure

the probabilistic interpretation of the spectra of evolving states, while the danger of possible couplings to uncontrollable ancillary systems is a far too abstract speculation to be of any physical importance in actual experimental contexts.

However, we have also seen that the true meaning of complete positivity can mainly be appreciated in relation to quantum entanglement of which it is just another facet. Quantum entanglement requires at least two systems, whereas, until recently, the literature on open quantum systems primarily has been dealing with single systems immersed in heat baths.

It appears then clear why the fundamental role of complete positivity does not emerge in full in usual open quantum system contexts. On the contrary, the whole perspective radically changes when one considers two systems in a same environment, as, for instance, two atoms in a heat bath at some finite temperature. The main point is that two such systems can be prepared in an entangled initial state; the usual unitary time-evolution is completely positive by its very construction and thus gentle to entangled states, while some dissipative time-evolution may not be completely positive and thus potentially conflicting with initial entangled states, making negative eigenvalues emerge in the course of the time-evolution.

More concretely, suppose the reduced dynamics of just one system S in the environment E to be given in terms of a semigroup of positive maps γ_t . Consider then two such systems (both denoted by S) embedded into E , without direct interaction between themselves. In first approximation, the states of the compound system $S + S$ will evolve according to the dissipative semigroups of maps $\Gamma_t \equiv \gamma_t \otimes \gamma_t$.

We stress the difference between the two contexts: the one just depicted, where the maps $\gamma_t \otimes \gamma_t$ describe the dynamics of two systems S in the same environment E , and the other, where the maps $\gamma_t \otimes \text{id}_A$ drive a single open quantum system S coupled to a remote and inert ancilla A that has nothing to do with it apart for possible statistical correlations (entanglement) in the initial state of $S + A$.

Suppose now that complete positivity is a mathematical artifact and may thus be dispensed with in actual physical contexts, where no ancilla effectively intervenes. Since we want that at least the positivity of the states be preserved, the crucial question is then the following:

Which are the conditions on γ_t such that $\Gamma_t = \gamma_t \otimes \gamma_t$ be positivity-preserving on the state-space of the open system $S + S$?

For n -level systems the answer is given by the following Theorem.⁸⁶

Theorem 3.3 *If a semigroup of positive maps γ_t acting on $\mathcal{S}(S)$ describes the dynamics of an n -level system S , then the semigroup $\Gamma_t = \gamma_t \otimes \gamma_t$ acting on $\mathcal{S}(S + S)$ is positivity-preserving if and only if γ_t is completely positive.*

The conclusion which is to be drawn from the previous theorem is the following. If γ_t is only positivity-preserving but not completely positive, then $\Gamma_t = \gamma_t \otimes \gamma_t$ can not be positivity-preserving. Therefore, there are states of $S + S$ whose spectrum does not remain positive under Γ_t and which thus lose their probabilistic interpretation.

tation in the course of time. Such states are necessarily entangled as Γ_t preserves in any case the positivity of separable states as in (37). In fact,

$$\Gamma_t[\rho_{sep}] = \sum_{ij} \lambda_{ij} \gamma_t[\rho_i^1] \otimes \gamma_t[\rho_j^2]$$

and γ_t is positivity-preserving by assumption. It is thus the existence of entangled states that makes the request of complete positivity necessary. As already observed, unitary time-evolutions are automatically completely positive, while dissipative semigroups are not in general and their physical consistency depends on the way Markov approximations are implemented.

Remarks 3.12

- (1) The argument of Theorem 3.3 gives a concrete explanation of why complete positivity is necessary by hinging on the necessity that at least the positivity of the time-evolution of bipartite systems be guaranteed. If $\Gamma_t = \gamma_t \otimes \gamma_t$ is positive, then γ_t must be completely positive and Γ_t is completely positive, too. Indeed, by using the Kraus-Stinespring representation (29), one checks that the composition of two completely positive maps is again in Kraus-Stinespring form, and thus completely positive. In the case above, $\Gamma_t = (\gamma_t \otimes \text{id}) \circ (\text{id} \otimes \gamma_t)$.
- (2) If one considers semigroups of maps of the form $\Gamma_t = \gamma_t^{(1)} \otimes \gamma_t^{(2)}$ with two different single-system semigroups, then Γ_t can be positivity preserving without $\gamma_t^{(1,2)}$ being both completely positive.⁸⁷ In this case, Γ_t is not completely positive; in fact, its generator has a Kossakowski matrix which consists of the orthogonal sum of those of the generators of $\gamma_t^{(1)}$ and $\gamma_t^{(2)}$, and one of them is not positive. Then, Γ_t is not robust against the coupling of $S + S$ to ancillas.
- (3) An important ingredient in the proof of Theorem 3.3 is time-continuity and the resulting existence of a generator; without continuity, there are counterexamples to its conclusions. For instance, take the transposition map \mathbb{T}_n , which can not be continuously connected to the identity. It is not completely positive, but it is easy to check that $\mathbb{T}_n \otimes \mathbb{T}_n$ is nevertheless a positive map.
- (4) With reference to the slippage of initial conditions argument briefly mentioned in Remark 3.10, its usage in the bipartite context would lead to argue that the transient effects prior to the Markovian regime are such that all entangled states dangerous to a semigroup of non-positive $\Gamma_t = \gamma_t \otimes \gamma_t$ should somehow be eliminated by the slippage operator. Such an operator might plausibly be constructed, but it would be adapted to the bipartite contexts; by going to multipartite systems it should then be re-adjusted, thus making the whole procedure become *ad hoc* and lose the general applicability it should possess.⁸³ \square

4. Open Quantum Systems and Entanglement Generation

In this Section we shall apply the results and considerations discussed so far to the study of a specific instance of open quantum system, that of atoms interacting

with a bath made of quantum fields. As we shall see, this model, besides having an intrinsic theoretical interest, underlays many phenomenological applications in chemistry, quantum optics and condensed matter physics.

As remarked before, the use of the open system paradigm in modelling specific physical situations requires an *a priori* unambiguous separation between subsystem and environment. In the weak coupling regime, this is typically achieved when the correlations in the environment decay much faster than the characteristic evolution time of the subsystem: in this case, the changes in the evolution of the subsystem occur on time-scales that are very long, so large that the details of the internal environment dynamics result irrelevant. It is precisely this “coarse grained” evolution that is captured by the Markovian master equations studied in Section 3.

Independent atoms immersed in external quantum fields and weakly coupled to them constitute one of the most common and interesting examples in which the open system paradigm finds its concrete realization. Indeed, in typical situations the differences between the atom internal energy levels ($\simeq \tau_S^{-1}$) result much smaller than the field correlation decay constants ($\simeq \tau_E^{-1}$) so that a clear distinction between subsystem, the non-interacting atoms, and environment, the external fields, is automatically achieved.

The atoms are usually treated in a non-relativistic approximation, as independent n -level systems, with zero size, while the environment is described by a set of quantum fields, often the electromagnetic field, in a given quantum state, typically either a temperature state or simply the vacuum state. The interaction of the fields with the atoms is taken to be of dipole type, a well justified approximation within the weak coupling assumption. Even in this simplified setting, that ignores all intricacies related to the internal atom structure and to the full coupling with the electromagnetic field, the model is of great relevance both theoretically and phenomenologically: indeed, with suitable adaptations, it is able to capture the main features of the dynamics of very different physical systems, like ions in traps, atoms in optical cavities and fibers, impurities in phonon fields (many concrete examples are presented in Refs.[1-16]).

Despite this ample range of possible applications and the attention devoted to it in the recent literature, no particular care is generally adopted in the various derivations of consistent subdynamics. As a result, time-evolutions that are not even positive, of the type discussed in Examples 3.3 and 3.8, have often been adopted in order to describe the subsystem physical properties: we have already pointed out that physical inconsistencies might be the outcome of such ill-defined dynamics.

As a relevant application of the theory of open quantum systems dynamics, in the following we shall explicitly derive and study in detail the reduced time-evolution obtained by tracing over the unobserved (infinite) field degrees of freedom. For simplicity, we shall restrict our attention to two-level atoms in interaction with a collection of independent, free, scalar fields in arbitrary d space-time dimensions, assumed to be in a state at temperature $T = 1/\beta$.

The time-evolution of a single atom will be first analyzed. Following the steps

outlined in Section 3, the weak coupling limit procedure will be adopted; it leads to a mathematically sound and physically consistent expression for the atom subdynamics in terms of completely positive quantum dynamical semigroups. Not surprisingly, the atom is found to be subjected to dissipative and decohering effects that asymptotically drive its state to an equilibrium configuration that is exactly thermal, at temperature T .

The case of a subsystem composed by more than one atom can be similarly treated. Again for simplicity we shall limit the discussion to the case of two, independent two-level atoms immersed in the same environment of thermal quantum fields. The corresponding master equation that, in the weak coupling limit, describes the reduced time-evolution of the atoms can be obtained by generalizing the techniques used in the single atom case. It again generates a semigroup of completely positive maps, that can be studied in detail. In particular, the asymptotic equilibrium state can be computed explicitly, and in general it turns out to be an entangled state of the two atoms, even in the case of a totally separable initial state.

This remarkable conclusion might appear at first sight rather surprising. As observed before, the interaction with an environment usually leads to decoherence and noise, mixing enhancing phenomena typically going against entanglement.

Example 4.1 As a drastic instance of mixing-enhancing behaviour, let us consider the so-called depolarizing channel affecting a two-level system; it is described by the following Kossakowski-Lindblad master equation

$$\partial_t \rho_t = \sigma_1 \rho_t \sigma_1 + \sigma_2 \rho_t \sigma_2 + \sigma_3 \rho_t \sigma_3 - 3\rho_t .$$

Its solution is $\rho_t = (1 - e^{-4t}) \mathbf{1}_2/2 + e^{-4t} \rho$, so that any initial state ρ , even a pure one, with zero von Neumann entropy, goes asymptotically into the totally depolarized state $\mathbf{1}_2/2$ with maximal entropy $\log 2$. \square

Since the closer to the totally depolarized state, the less entangled a state is, one generally expects that when a bipartite system is immersed in an environment, quantum correlations that might have been created before by a direct interaction between the two subsystems actually disappear. And this could occur even in finite time.^{88,58} The degrading of entanglement by an external environment is clearly a curse in quantum information, where one tries to maintain quantum correlations long enough to complete a quantum computation. Various error correcting strategies have been devised precisely to counteract environment decoherence.¹⁸

However, an external environment can also provide an indirect interaction between otherwise totally decoupled subsystems and therefore a means to correlate them.^{89,90,91,92} This phenomenon has been first established in exactly solvable models: there, correlations between the two subsystems take place during a short time transient phase, where the reduced dynamics of the subsystems contains memory effects.

Remarkably, entanglement generation may occur also in the long time, Markovian regime, through a purely noisy mechanism:⁹³ it is precisely this situation that

is relevant in the analysis of the dynamics of two independent atoms interacting with the same vacuum quantum field.

4.1. *Single Atom Systems: Master Equation*

We shall first deal with a single atom in weak interaction with a collection of free scalar fields at temperature T , in d space-time dimensions. As mentioned before, we are not interested in the details of the atom internal dynamics. We shall therefore model it, in a nonrelativistic way, as a simple two-level system, which can be fully described in terms of a two-dimensional Hilbert space.

In absence of any interaction with the external scalar fields, the atom internal dynamics will be driven by a 2×2 Hamiltonian matrix H_S , that in the chosen basis can be taken to assume the most general form (*cf.* Examples 2.2, 3.1)

$$H_S = \frac{\omega}{2} \vec{n} \cdot \vec{\sigma} , \quad (161)$$

where σ_i , $i = 1, 2, 3$ are again the Pauli matrices, n_i , $i = 1, 2, 3$ are the components of a unit vector, while ω represents the gap between the two energy eigenvalues.

To conform with the standard open system paradigm (see (17)), the interaction of the atom with the external scalar fields is assumed to be weak and described by a Hamiltonian H' that is linear in both atom and field variables:

$$H' = \sum_{i=1}^3 \sigma_i \otimes \Phi_i(x) . \quad (162)$$

As the atom is taken to be an idealized point-particle, without size (see Remark 4.1.2 below), the interaction is effective only at the atom position x^μ , $\mu = 0, 1, \dots, d$, that, without loss of generality, can be chosen to be the origin of the reference frame. As a consequence, all coordinates vanish, $x^\mu = 0$, $\mu = 1, 2, \dots, d$, except for the time variable, $x^0 \equiv t$. The operators Φ represent the external quantum fields, and are taken to be spinless and massless for simplicity. They evolve in time as free relativistic fields with an Hamiltonian H_Φ whose explicit expression need not be specified in detail. Further, we shall assume the atom and the fields to be prepared at time $t = 0$ in an uncorrelated state, with the fields in the temperature state ρ_β , as in (105), and the atom in a generic initial state $\rho(0)$.

Example 4.2 Although apparently very simplified, the model presented above is of relevance in various phenomenological applications. As an instance, let us discuss the case of a two-level atom in interaction with the electromagnetic field in an optical fiber through the standard dipole coupling.⁹⁴ In this case, working in three-dimensional space, the interaction Hamiltonian takes the form:

$$H' = -\vec{d} \cdot \vec{E}(\vec{x}) , \quad (163)$$

where \vec{d} denotes the operator representing the atom dipole moment, while \vec{E} is the electric field at the atom position \vec{x} .

In absence of the field, the atom dynamics can again be taken to be driven by the generic two-level Hamiltonian (161), with eigenstates $|-\rangle$ and $|+\rangle$, while the electromagnetic field is quantized using the Maxwell action:

$$\mathcal{S} = -\frac{1}{4} \int d^3\vec{x} dt F_{\mu\nu} F^{\mu\nu} , \quad (164)$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the field strength expressed in terms of the electromagnetic 4-vector potential A_μ . Without loss of generality, we shall choose to work in the familiar $A_0 = 0$ gauge, so that only the vector potential \vec{A} will be relevant.

Since the dipole moment \vec{d} is a vector operator with odd parity, one finds: $\langle -|\vec{d}|-\rangle = \langle +|\vec{d}|+\rangle = 0$. Furthermore, one can write:

$$\langle +|\vec{d}|-\rangle = \langle -|\vec{d}|+\rangle^* = |\vec{d}| e^{i\theta} \vec{u} , \quad (165)$$

where \vec{u} is the unit vector that defines the orientation of the atom in space, while θ is a phase. As a consequence, the representation of the operator \vec{d} on the two-dimensional atom Hilbert space has vanishing diagonal elements, so that one can rewrite (163) as:

$$H' = -|\vec{d}| E(\vec{x}) \left[e^{i\theta} \sigma_+ + e^{-i\theta} \sigma_- \right] , \quad (166)$$

where $E(\vec{x}) \equiv \vec{u} \cdot \vec{E}(\vec{x})$ and $\sigma_\pm = \sigma_1 \pm i\sigma_2$. Further, note that the phase θ can be reabsorbed into a redefinition of the Pauli matrices, $\sigma_\pm \rightarrow e^{\mp i\theta} \sigma_\pm$, without affecting their algebraic properties; in other terms, there is no loss of generality in setting θ to zero.

Let us now exploit the fact that the atom is inserted in an optical fiber. One can always choose the direction along the fiber to coincide with the z -axis, the x - and y -axis representing the corresponding transverse directions. The spatial geometry becomes essentially unidimensional and the vector potential \vec{A} can be taken to be independent from the x and y coordinates. Moreover, in such a geometry the electromagnetic energy flows along the fiber and thus only the components of \vec{A} transverse to the fiber are non-vanishing; further, of these only $A \equiv \vec{u} \cdot \vec{A}$ really couples to the atom.

Taking into account all these conditions, the Maxwell action (164) reduces to

$$\mathcal{S} = \frac{\Sigma}{2} \int dt dz \left[\partial_t A \partial_t A - \partial_z A \partial_z A \right] , \quad (167)$$

where $\Sigma = \int dx dy$ is the cross section area of the fiber. By further noting that $E = -\partial_t A$ and by introducing the dimensionless rescaled field $\phi(t, z) = A(t, z)\sqrt{\Sigma}$, the interaction Hamiltonian (166) can be rewritten as:

$$H' = \lambda \partial_t \phi(0, z) \left[\sigma_+ + \sigma_- \right] , \quad (168)$$

where $\lambda = |\vec{d}|/\sqrt{\Sigma}$ plays the role of coupling constant. It is precisely of the form (162), with $\Phi_1 = \partial_t \phi$ and $\Phi_2 = \Phi_3 = 0$, where ϕ is a 1+1-dimensional free, massless

scalar field; its dynamics is generated by the Hamiltonian H_ϕ that corresponds to the action (167):

$$H_\phi = \frac{1}{2} \int dt dz \left[(\partial_t \phi)^2 + (\partial_z \phi)^2 \right]. \quad (169)$$

The scattering theory for atoms in an optical fiber described by interactions of the form (168) has been discussed in Refs.[95, 96] by means of a formal mapping to the anisotropic Kondo model. Here instead we are interested in analyzing the full reduced dynamics of the atom and not only its asymptotic properties. We shall do it by turning to the more general interacting Hamiltonian in (162). \square

The total Hamiltonian H describing the complete system, the two-level atom together with the external fields Φ_i , can thus be written as

$$H = H_S \otimes \mathbf{1}_\Phi + \mathbf{1}_S \otimes H_\Phi + \lambda H'. \quad (170)$$

It is precisely of the form discussed in the previous Section, with centered environmental operators, $\text{Tr}[\rho_\beta \Phi_i] = 0$. It generates the time-evolution of the total density matrix ρ_{tot} , via the Hamiltonian equation

$$\frac{\partial \rho_{\text{tot}}(t)}{\partial t} = \mathbb{L}_H^\lambda[\rho_{\text{tot}}(t)], \quad (171)$$

starting at $t = 0$ from the initial configuration: $\rho_{\text{tot}}(0) = \rho(0) \otimes \rho_\beta$. As explained before, we want to follow the dynamics of the reduced density matrix $\rho(t) \equiv \text{Tr}_\Phi[\rho_{\text{tot}}(t)]$ on time-scales that are long with respect to the decay time of correlations in the environment. This can be obtained by suitably rescaling the time variable, $t \rightarrow t/\lambda^2$ and then taking the limit $\lambda \rightarrow 0$, following the mathematically precise procedure of the *weak coupling limit* discussed in Section 3.3.2.

The resulting master equation for $\rho(t)$ takes a Kossakowski-Lindblad form (49)

$$\frac{\partial \rho(t)}{\partial t} = -i[H_{\text{eff}}, \rho(t)] + \mathbb{D}[\rho(t)], \quad (172)$$

with \mathbb{D} as in (50). The effective Hamiltonian H_{eff} and the coefficients of the 3×3 Kossakowski matrix C_{ij} that appear in (50) are determined by the Fourier transform of the field correlations:

$$h_{ij}(\zeta) = \int_{-\infty}^{+\infty} dt e^{i\zeta t} \langle \Phi_i(t) \Phi_j(0) \rangle. \quad (173)$$

Since the fields are independent and assumed to obey a free evolution, one finds:

$$\langle \Phi_i(x) \Phi_j(y) \rangle \equiv \text{Tr}[\Phi_i(x) \Phi_j(y) \rho_\beta] = \delta_{ij} G_\beta(x - y), \quad (174)$$

where $G_\beta(x - y)$ is the standard d -dimensional Wightmann function for a single massless relativistic scalar field in a state at inverse temperature β .⁹⁷ With the proper $i\varepsilon$ prescription, it can be written as:

$$G_\beta(x) = \int \frac{d^d k}{(2\pi)^{d-1}} \theta(k^0) \delta(k^2) \left[(1 + \mathcal{N}_\beta(k^0)) e^{-ik \cdot x} + \mathcal{N}_\beta(k^0) e^{ik \cdot x} \right] e^{-\varepsilon k^0}, \quad (175)$$

where

$$\mathcal{N}_\beta(k^0) = \frac{1}{e^{\beta k^0} - 1} . \quad (176)$$

Its Fourier transform can be readily evaluated:

$$\mathcal{G}_\beta(\zeta) = \int_{-\infty}^{+\infty} dt e^{i\zeta t} G_\beta(t) = \left[\frac{2|\zeta|^{d-2}}{(4\pi)^{\frac{d-1}{2}} \Gamma\left(\frac{d-1}{2}\right)} \right] \frac{\pi}{\zeta} \frac{1}{1 - e^{-\beta\zeta}} . \quad (177)$$

Remarks 4.1

- (1) As mentioned in Remark 3.7.3, the convergence in the *weak coupling limit* of the evolution equation for the reduced density matrix $\rho(t)$ to the Markovian limit (172) stems from the asymptotic behavior of the two-point function $G_\beta(t) \equiv G_\beta(t, \vec{0})$ for large t (see, (135)). More precisely, the combination $|G_\beta(t)|(1+t)^\eta$ should be integrable on the positive half real line, for some $\eta > 0$. In the case of a massless field, the integrals in (175) can be expressed in terms of the standard Poly-Gamma function, $\psi^{(n)}(z) = d^{n+1} \log \Gamma(z)/dz^{n+1}$; explicitly, one finds:⁶⁸

$$G_\beta(t) = \frac{1}{(4\pi)^{\frac{d-1}{2}} \Gamma\left(\frac{d-1}{2}\right)} \left\{ \frac{2}{(-\beta)^{d-2}} \operatorname{Re} \left[\psi^{(d-3)} \left(\frac{\varepsilon - it}{\beta} \right) \right] - \frac{(d-3)!}{(\varepsilon - it)^{d-2}} \right\} . \quad (178)$$

Since $\psi^{(n)}(z) \sim 1/z^n$ for $|z| \rightarrow \infty$, $\operatorname{Arg}(z) < \pi$, $G_\beta(t)$ behaves like $1/t^{d-3}$ for large t in $d > 4$, while for $d = 4$ it falls off as $1/t^2$ due to a cancellation arising from taking the real part of $\psi^{(1)}$ in (178). Therefore, the conditions for the existence of the *weak coupling limit* are assured, at infinity by the fall off of $G_\beta(t)$, provided $d \geq 4$, and at zero by the $i\varepsilon$ prescription.¹ Notice that in two dimensions (178) gives a logarithmic behaviour for the two point function, so that in general the *weak coupling limit* is not guaranteed to exist. The limit is however well-defined for an atom in an optical fiber as discussed in Example 4.1. There, the field operators Φ that couple with the atom variables involve the time derivative of a two-dimensional, free, massless scalar field; as a consequence, the relevant environment correlation $\langle \Phi(t)\Phi(0) \rangle$ actually behaves as $\partial_t^2 G_\beta(t)$, and integrability at infinity is still assured.

- (2) The $i\varepsilon$ prescription involved in the definition of the Wightmann function (175) originates from causality requirements. In the present setting, it can be alternatively interpreted as an infinitesimal remnant of the size of the atom.⁹⁹ Indeed, assume that the atom has a spatial extension, with a profile given by a function $f(\vec{x})$. Since the atom-field interaction takes now place on the whole region

¹In four-dimensional spacetime, the asymptotic behaviour for large space-like separation of the two-point Wightmann function has been studied in Ref.[98] in the case of arbitrary interacting fields. In general, $G_\beta(t)$ is found to fall off at infinity as $1/t^{3/2}$, so that the *weak coupling limit* is assured to exist even in this very general setting.

occupied by the atom, the field operator entering the Hamiltonian H' in (162) is now smeared out over the atom size,

$$\Phi_i(t) = \int d^{d-1}x f(\vec{x}) \Phi_i(t, \vec{x}) , \quad (179)$$

instead of being just $\Phi_i(t, \vec{0})$, *i.e.* evaluated at the atom position. As a consequence, the correlation function (174) involves the Fourier transform $\hat{f}(\vec{k}) = \int d^{d-1}x e^{i\vec{k}\cdot\vec{x}} f(\vec{x})$ of the shape function. As an illustration, assume the fields to be in the vacuum, zero-temperature state; then, (compare with (175)):

$$\langle \Phi_i(t) \Phi_j(0) \rangle = \delta_{ij} \int \frac{d^{d-1}k}{(2\pi)^{d-1}} \frac{1}{2|\vec{k}|} |\hat{f}(\vec{k})|^2 e^{-i|\vec{k}|t} . \quad (180)$$

Since at the end we want to model a point-like atom, we choose a shape function approximating a $(d-1)$ -dimensional δ -function:

$$f(\vec{x}) = \prod_{i=1}^{d-1} \frac{1}{2\pi} \frac{\varepsilon}{[(x_i)^2 + (\varepsilon/2)^2]^2} , \quad \varepsilon > 0 ; \quad (181)$$

in this way, the atom is viewed as $d-1$ -dimensional box with size ε . The Fourier transform of (181) can be easily computed: $\hat{f}(\vec{k}) = e^{-|\vec{k}|\varepsilon/2}$; inserting this result in (180), one readily recovers the standard $i\varepsilon$ prescription for the field correlations. \square

As discussed in Section 3.3.2, the explicit expression of the Kossakowski matrix C_{ij} involves a sum over the differences of the energy levels of the system Hamiltonian H_S , here just $\pm\omega/2$; it corresponds to the decomposition of the system operators σ_i along the two energy eigenprojectors

$$P_{\pm} = \frac{1}{2}(\mathbf{1}_2 \pm \vec{n} \cdot \vec{\sigma}) , \quad (182)$$

as indicated in (127), namely:

$$\sigma_i(0) = P_+ \sigma_i P_+ + P_- \sigma_i P_- , \quad \sigma(\pm) = P_{\pm} \sigma_i P_{\mp} . \quad (183)$$

The 2×2 auxiliary matrices $\sigma_i(0)$, $\sigma_i(+)$ and $\sigma_i(-)$ can be further decomposed along the Pauli matrices themselves,

$$\sigma_i(\xi) = \sum_{j=1}^3 \psi_{ij}^{(\xi)} \sigma_j , \quad \text{for } \xi = +, -, 0 , \quad (184)$$

with the help of the three-dimensional tensor coefficients

$$\psi_{ij}^{(0)} = n_i n_j , \quad \psi_{ij}^{(\pm)} = \frac{1}{2}(\delta_{ij} - n_i n_j \pm i\epsilon_{ijk} n_k) . \quad (185)$$

Recalling (173), one can then write (compare with (133)):

$$C_{ij} = \sum_{\xi=0,\pm} \sum_{k,l=1}^3 h_{kl}(\xi\omega) \psi_{ki}^{(\xi)} \psi_{lj}^{(-\xi)} \quad (186)$$

$$= \mathcal{G}_\beta(0) \psi_{ij}^{(0)} + \mathcal{G}_\beta(\omega) \psi_{ij}^{(-)} + \mathcal{G}_\beta(-\omega) \psi_{ij}^{(+)} , \quad (187)$$

where the second line follows from the property: $\sum_{k=1}^3 \psi_{ki}^{(\xi)} \psi_{kj}^{(-\xi)} = \psi_{ij}^{(-\xi)}$. One can easily check that, being the sum of three positive matrices, the matrix C_{ij} is also positive, so that the dynamical semigroup generated by (172) consists of completely positive maps. As discussed before, this is to be expected, since (187) is the result of the *weak coupling limit*, in the mathematically well-defined formalism developed in Section 3.3.2. On the other hand, let us remark once more, that direct use of the standard second order perturbative approximation (as adopted for example in Ref.[100]) leads to physically inconsistent results, giving a finite time-evolution for $\rho(t)$ that in general does not preserve the positivity of probabilities.

Example 4.3 As an explicit illustration of this general framework, it is instructive to reconsider the simple system discussed in Example 3.3, and analyze its dynamics in the long-time, Markovian regime using the techniques just presented. The model describes the behaviour of a two-level atom immersed in a one-dimensional boson gas at temperature β^{-1} , that in the thermodynamical limit can be fully described in terms of a two-dimensional, free, massless scalar field.

Positioning the atom at the origin, the total Hamiltonian in (81) can then be conveniently rewritten as:

$$H = \frac{\Omega}{2} \sigma_3 \otimes \mathbf{1}_\phi + \mathbf{1}_S \otimes H_\phi + \lambda \sigma_3 \otimes \partial_t \phi(0) , \quad (188)$$

so that we are precisely in the condition of Eq. (161) and (162) with $\vec{n} = (0, 0, 1)$ and $\Phi_1 = \Phi_2 = 0$, $\Phi_3 = \partial_t \phi$. The Fourier transform of the bath correlation functions, $G_\beta(t) = \text{Tr}[\partial_t \phi(t) \partial_t \phi(0) \rho_\beta]$, can be easily evaluated:

$$\mathcal{G}_\beta(\zeta) = \frac{\zeta}{1 - e^{-\beta\zeta}} ; \quad (189)$$

through (186), one then obtains the expression for the Kossakowski matrix C_{ij} . It turns out that only the entry C_{33} is actually nonvanishing. As a consequence, the Markovian master equation describing the reduced dynamics of the two-level system takes, in the interaction picture, the particularly simple form:

$$\partial_t \rho(t) = \frac{\lambda^2}{2\beta} [\sigma_3 \rho(t) \sigma_3 - \rho(t)] . \quad (190)$$

In the basis of eigenvectors of σ_3 , $\sigma_3|i\rangle = (-1)^{i+1}|i\rangle$, $i = 0, 1$, one then recovers the exponential damping of the off-diagonal entries of $\rho(t)$ already discussed in Example 3.3:

$$\begin{aligned} \langle i|\rho(t)|i\rangle &= \langle i|\rho(0)|i\rangle , \\ \langle 1|\rho(t)|0\rangle &= e^{-2\lambda^2 t/\beta} \langle 1|\rho(0)|0\rangle . \end{aligned} \quad (191)$$

Although in a simplified settings, this result constitutes a direct evidence that the Markovian master equation (190), obtained using the mathematically well defined *weak coupling limit* procedure, correctly reproduces the long time behaviour of the exact reduced dynamics. \square

The Lamb shift correction $H_E^{(2)}$ to the effective Hamiltonian $H_{\text{eff}} = H_S + H_E^{(2)}$ can be similarly computed. It involves the Hilbert transform of the correlations (173), as indicated in (131) and (132). In practice, recalling (174), it can be expressed in terms of the following integral transform of the scalar Wightmann function

$$\mathcal{K}_\beta(\zeta) = \frac{\mathcal{P}}{i\pi} \int_{-\infty}^{\infty} dz \frac{\mathcal{G}_\beta(z)}{z - \zeta} . \quad (192)$$

Explicitly, one finds:

$$H_E^{(2)} = \frac{1}{2} \sum_{i,j,k=1}^3 \epsilon_{ijk} \left[\mathcal{K}_\beta(\omega) \psi_{jk}^{(-)} + \mathcal{K}_\beta(-\omega) \psi_{jk}^{(+)} \right] \sigma_i . \quad (193)$$

Remark 4.2 This result deserves a closer look. Recalling (177), the definition of $\mathcal{K}_\beta(\zeta)$ in (192) can be split as:

$$\mathcal{K}_\beta(\zeta) = \frac{2}{i(4\pi)^{\frac{d-1}{2}} \Gamma\left(\frac{d-1}{2}\right)} \left[\mathcal{P} \int_0^\infty dz \frac{z^{d-3}}{z - \zeta} \right. \quad (194)$$

$$\left. + \mathcal{P} \int_0^\infty dz \frac{z^{d-3}}{1 - e^{\beta z}} \left(\frac{1}{z + \zeta} - \frac{1}{z - \zeta} \right) \right] , \quad (195)$$

into a vacuum and a temperature-dependent piece. Although not expressible in terms of elementary functions, the temperature dependent second term is a finite, odd function of ζ , vanishing as β becomes large, *i.e.* in the limit of zero temperature. The first contribution in (194) is however divergent for $d \geq 3$. As a consequence, despite some cancellations that occur in (193) (see below), the Lamb contribution $H_E^{(2)}$ turns out in general to be infinite, and its definition requires the introduction of a suitable cutoff and a renormalization procedure.

This is a well known fact, and has nothing to do with the weak coupling assumptions used in deriving the master equation. Rather, the appearance of the divergences is due to the non-relativistic treatment of the two-level atom, while any sensible calculation of energy shifts would require quantum field theory techniques.¹⁰¹

In our quantum mechanical setting, the procedure needed to make the Lamb contribution $H_E^{(2)}$ well defined is therefore clear: perform a suitable temperature independent subtraction, so that the expression in (193) reproduces the correct quantum field theory result, obtained by considering the field in its vacuum state. \square

4.2. Single Atom Dynamics and Decoherence

From now on we shall work in ordinary four-dimensional Minkowski spacetime and therefore specialize $d = 4$. In this case, the Kossakowski matrix C_{ij} in (187) takes the general form

$$C_{ij} = A \delta_{ij} - iB \epsilon_{ijk} n_k + C n_i n_j , \quad (196)$$

where the quantities A , B and C depend on the system frequency ω and the inverse temperature β :

$$A = \frac{1}{2} [\mathcal{G}_\beta(\omega) + \mathcal{G}_\beta(-\omega)] = \frac{\omega}{4\pi} \left[\frac{1 + e^{-\beta\omega}}{1 - e^{-\beta\omega}} \right] , \quad (197)$$

$$B = \frac{1}{2} [\mathcal{G}_\beta(\omega) - \mathcal{G}_\beta(-\omega)] = \frac{\omega}{4\pi} , \quad (198)$$

$$C = \frac{1}{2} [2\mathcal{G}_\beta(0) - \mathcal{G}_\beta(\omega) - \mathcal{G}_\beta(-\omega)] = \frac{\omega}{4\pi} \left[\frac{2}{\beta\omega} - \frac{1 + e^{-\beta\omega}}{1 - e^{-\beta\omega}} \right] . \quad (199)$$

On the other hand, the effective Hamiltonian H_{eff} can be rewritten as

$$H_{\text{eff}} = \frac{\tilde{\omega}}{2} \vec{n} \cdot \vec{\sigma} , \quad (200)$$

in terms of a redefined frequency:

$$\tilde{\omega} = \omega + i [\mathcal{K}_\beta(-\omega) - \mathcal{K}_\beta(\omega)] . \quad (201)$$

Remark 4.3 As explained above, a suitable temperature independent subtraction has been implicitly included in the definition of the combination $\mathcal{K}(-\omega) - \mathcal{K}(\omega)$, which otherwise would have been logarithmically divergent (compare with the expression in (194)). It comes from a “mass” renormalization due to virtual vacuum effects of the full relativistic theory,¹⁰¹ and can not be accounted for by a mere frequency shift, as the expression (201) might erroneously suggest. \square

In order to discuss explicitly the properties of the solutions of the master equation (172), it is convenient to decompose the density matrix ρ in terms of the Pauli matrices, as introduced in Example 3.1:

$$\rho = \frac{1}{2} (\mathbf{1}_2 + \vec{\rho} \cdot \vec{\sigma}) . \quad (202)$$

Then, as shown there, the evolution equation (172) can be rewritten as a Schrödinger-like equation for the coherence (Bloch) vector $|\rho(t)\rangle$ of components $(1, \rho_1(t), \rho_2(t), \rho_3(t))$:

$$\frac{\partial}{\partial t} |\rho(t)\rangle = -2 (\mathcal{H} + \mathcal{D}) |\rho(t)\rangle . \quad (203)$$

The 4×4 matrices \mathcal{H} and \mathcal{D} correspond to the Hamiltonian and dissipative contributions, respectively; they can be parametrized as in Example 3.1, Eqs.(53) and (54), in terms of the quantities $\omega_i = (\tilde{\omega}/2) n_i$, $i = 1, 2, 3$, coming from H_{eff} , $u = -4B n_1$,

$v = -4B n_2$, $w = -4B n_3$, coming from the imaginary part of the Kossakowski matrix (196), and

$$a = 2A + C(n_2^2 + n_3^2), \quad b = -C n_1 n_2, \quad (204)$$

$$\alpha = 2A + C(n_1^2 + n_3^2), \quad c = -C n_1 n_3, \quad (205)$$

$$\gamma = 2A + C(n_1^2 + n_2^2), \quad \beta = -C n_2 n_3, \quad (206)$$

coming from its real part. The 3×3 , symmetric submatrix $\mathcal{D}^{(3)}$ defined in (56) with these last six parameters as entries, is manifestly positive; its eigenvalues are in fact $\lambda_1 = 2A$ and $\lambda_{\pm} = 2A + C$. As a consequence, for large times $|\rho(t)\rangle$ reaches a unique equilibrium state $|\rho_{eq}\rangle$.¹⁰² This asymptotic state is determined by the condition $(\mathcal{H} + \mathcal{D})|\rho_{eq}\rangle = 0$, and therefore is obtained by inverting $\mathcal{D}^{(3)}$:

$$|\rho_{eq}\rangle = \{1, -R n_1, -R n_2, -R n_3\}, \quad R \equiv \frac{B}{A} = \frac{1 - e^{-\beta\omega}}{1 + e^{-\beta\omega}}. \quad (207)$$

Inserting these components in the expansion (202), one finds that the asymptotic density matrix ρ_{eq} is a thermal state in equilibrium with the field environment at the latter temperature $T = 1/\beta$,

$$\rho_{eq} = \frac{e^{-\beta H_S}}{\text{Tr}[e^{-\beta H_S}]} . \quad (208)$$

This asymptotic thermalization phenomenon is just one of the many effects that the dissipative dynamics generated by (203) produces on the two-level atom. More details on the thermalization process can be retrieved by studying the behaviour of the atom state $\rho(t)$ for finite times; it is formally given by the exponentiation of (203):

$$|\rho(t)\rangle = e^{-2(\mathcal{H} + \mathcal{D})t} |\rho(0)\rangle . \quad (209)$$

Recalling the definition (4), the evolution in time of any relevant atom observable, a Hermitian 2×2 matrix X , can thus be explicitly computed:

$$\langle X(t) \rangle = \text{Tr}[X \rho(t)] . \quad (210)$$

When the observable X represents itself an admissible atom state ρ_f , the mean value (210) coincides with the probability $\mathcal{P}_{i \rightarrow f}(t)$ that the evolved atom density matrix $\rho(t)$, initially in $\rho(0) \equiv \rho_i$, be found in such a state at time t . Using (209), this probability can be computed explicitly:

$$\begin{aligned} \mathcal{P}_{i \rightarrow f}(t) = & \frac{1}{2} \left\{ 1 - (\vec{\rho}_f \cdot \vec{n}) \left(1 - e^{-4At} \right) \left[\frac{1 - e^{-\beta\omega}}{1 + e^{-\beta\omega}} \right] + e^{-4At} (\vec{\rho}_i \cdot \vec{n}) (\vec{\rho}_f \cdot \vec{n}) \right. \\ & \left. + e^{-2(2A+C)t} \left(\left[(\vec{\rho}_i \cdot \vec{\rho}_f) - (\vec{\rho}_i \cdot \vec{n}) (\vec{\rho}_f \cdot \vec{n}) \right] \cos \tilde{\omega}t - \vec{n} \cdot (\vec{\rho}_i \times \vec{\rho}_f) \sin \tilde{\omega}t \right) \right\} . \end{aligned} \quad (211)$$

In the above expression, we have expanded the density matrices ρ_i , ρ_f as in (202) and used the notations $(\vec{\rho}_i \cdot \vec{\rho}_f)$ and $(\vec{\rho}_i \times \vec{\rho}_f)$ (and similarly with \vec{n}) to represent

scalar and vector products of their corresponding three-dimensional coherence vectors. As expected, this expression contains exponentially decaying factors involving the eigenvalues λ_1 and λ_{\pm} defined earlier, modulated by oscillating terms in the effective frequency $\tilde{\omega}$. In other terms, the two-level atom immersed in scalar fields at temperature $1/\beta$ is subjected to decoherence and dissipation, both effects being governed by the Planckian factors appearing in the Kossakowski matrix (196)-(199).

When $\vec{\rho}_i = -\vec{n}$ and $\vec{\rho}_f = \vec{n}$, the density matrices ρ_i, ρ_f represent the ground and excited states of the system Hamiltonian H_S in (161). In this case, the expression in (211) simplifies,

$$\mathcal{P}_{i \rightarrow f}(t) = \frac{1}{1 + e^{\beta\omega}} \left(1 - e^{-4At} \right), \quad (212)$$

giving the probability for a spontaneous transition of the atom from the ground state to its excited state. Note that this phenomenon of spontaneous excitation disappears as $\beta \rightarrow \infty$, *i.e.* when the environment is at zero temperature.

Remark 4.4 Although the behaviour of $\mathcal{P}_{i \rightarrow f}(t)$ in (211) and (212) is in principle experimentally observable through the use of suitable interferometric devices, in the study of the behaviour of atoms in optical cavities one often limits the discussion to the spontaneous excitation rate $\Gamma_{i \rightarrow f}$, the probability per unit time of the transition $i \rightarrow f$, in the limit of an infinitely slow switching on and off of the atom-field interaction. In our formalism, its expression can be easily obtained by taking the time derivative of $\mathcal{P}_{i \rightarrow f}(t)$ at $t = 0$; in the case of (212), one then finds

$$\Gamma_{i \rightarrow f} = \frac{\omega}{\pi} \frac{1}{e^{\beta\omega} - 1}. \quad (213)$$

□

4.3. Two Atoms: Environment Induced Entanglement Generation

We have thus far analyzed the dynamics of an atom immersed in a bath of scalar massless fields at finite temperature, and found that, through decoherence effects, the atom state is driven towards a purely thermal equilibrium state, characterized by the same field temperature. When the subsystem in interaction with the field environment consists of two, non-interacting two-level atoms one thus expects similar mixing-enhancing phenomena to occur, leading in particular to loss of the mutual quantum correlation (entanglement) that might have been present at the beginning.

However, even though not directly coupled, the external field through which the two atoms move may provide an indirect interaction between them, and thus a means to entangle them. Indeed, entanglement generation through the action of an external heat bath has been shown to occur in certain circumstances; it is therefore of physical interest to investigate the same issue also in the present physical situation.

We shall therefore start by considering a system composed by two, equal two-level atoms, that start interacting with the external fields at time $t = 0$. Being independent, without direct mutual interaction, their internal dynamics can again be taken to be described by the generic Hamiltonian (161). Then, the total two-system Hamiltonian H_S is now the sum of two terms:

$$H_S = H_S^{(1)} + H_S^{(2)} , \quad H_S^{(1)} = \frac{\omega}{2} \sum_{i=1}^3 n_i (\sigma_i \otimes \mathbf{1}) , \quad H_S^{(2)} = \frac{\omega}{2} \sum_{i=1}^3 n_i (\mathbf{1} \otimes \sigma_i) . \quad (214)$$

Similarly, being immersed in the same set of free fields and within the weak coupling hypothesis, the atom-field interaction Hamiltonian can be most simply assumed to be the generalization of that in (162):

$$H' = \sum_{i=0}^3 \left[(\sigma_i \otimes \mathbf{1}) \otimes \Phi_i(x) + (\mathbf{1} \otimes \sigma_i) \otimes \Psi_i(x) \right] . \quad (215)$$

On the other hand, the Hamiltonian describing the environment dynamics remains that of a collection of free, independent scalar fields Φ_i and Ψ_i .

Remark 4.5 In writing the interaction terms in (215), we have assumed the two atoms to interact with the field bath through two different field operators, Φ and Ψ , respectively; as we shall see, this allows discussing entanglement generation in a more general setting. For two equal atoms, the identification $\Phi = \Psi$ is however physically justified, and we shall adopt it in most of the following analysis. On the other hand, since the two atoms are assumed to be pointlike, with infinitesimal size, there is no restriction in positioning them at the same point x , and the coupling in H' precisely reflects this simplified assumption.^m \square

The derivation of the appropriate master equation describing the dynamics of the two atoms proceeds as in the case of a single atom, discussed in the previous Section. One starts from the Liouville-von Neumann equation (171) generating the time-evolution of the state $\rho_{\text{tot}}(0)$ of the total system {atoms + external fields}, and then traces over the fields degrees of freedom, assuming a factorized initial state $\rho_{\text{tot}}(0) = \rho(0) \otimes \rho_\beta$. In the *weak coupling limit*, the two-atom system state $\rho(t)$, now a 4×4 density matrix, is seen evolving in time according to a quantum dynamical semigroup of completely positive maps, generated by a master equation in Kossakowski-Lindblad form:

$$\frac{\partial \rho(t)}{\partial t} = -i[\mathcal{H}_{\text{eff}}, \rho(t)] + \mathbb{D}[\rho(t)] . \quad (216)$$

The unitary term depends on an effective Hamiltonian which is the sum of H_S in (214) and suitable Lamb contributions: $\mathcal{H}_{\text{eff}} = H_{\text{eff}}^{(1)} + H_{\text{eff}}^{(2)} + H_{\text{eff}}^{(12)}$. The first

^mThe case of spacially separated atoms can also be similarly treated, adopting the same open system techniques; for details, see Ref.[103].

two represent single system contributions; they can be written as in (214), but in general with different terms for the two atoms:

$$H_{\text{eff}}^{(1)} = \sum_{i=1}^3 H_i^{(1)}(\sigma_i \otimes \mathbf{1}) , \quad H_{\text{eff}}^{(2)} = \sum_{i=1}^3 H_i^{(2)}(\mathbf{1} \otimes \sigma_i) . \quad (217)$$

The third piece is a field-generated direct two-atom coupling term, that in general can be written as:

$$H_{\text{eff}}^{(12)} = \sum_{i,j=1}^3 H_{ij}^{(12)}(\sigma_i \otimes \sigma_j) . \quad (218)$$

As in the single atom case, a suitable temperature-independent renormalization procedure needs to be implemented in order to make all these contributions well defined.

The dissipative contribution $\mathbb{D}[\rho(t)]$ can be written as in (49),

$$\mathbb{D}[\rho] = \sum_{\alpha,\beta=1}^6 C_{\alpha\beta} \left[\mathcal{F}_\beta \rho \mathcal{F}_\alpha - \frac{1}{2} \left\{ \mathcal{F}_\alpha \mathcal{F}_\beta, \rho \right\} \right] , \quad (219)$$

with the help of the matrices $\mathcal{F}_\alpha = \sigma_\alpha \otimes \mathbf{1}$ for $\alpha = 1, 2, 3$, $\mathcal{F}_\alpha = \mathbf{1} \otimes \sigma_{\alpha-3}$ for $\alpha = 4, 5, 6$. The Kossakowski matrix $C_{\alpha\beta}$ is now a positive 6×6 matrix, that can be represented as

$$C = \begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{B}^\dagger & \mathcal{C} \end{pmatrix} , \quad (220)$$

by means of the 3×3 matrices $\mathcal{A} = \mathcal{A}^\dagger, \mathcal{C} = \mathcal{C}^\dagger$ and \mathcal{B} . In terms of this decomposition, $\mathbb{D}[\rho]$ can be rewritten in the following more explicit form:

$$\begin{aligned} \mathbb{D}[\rho] = & \sum_{i,j=1}^3 \left(\mathcal{A}_{ij} \left[(\sigma_j \otimes \mathbf{1}) \rho (\sigma_i \otimes \mathbf{1}) - \frac{1}{2} \left\{ (\sigma_i \sigma_j \otimes \mathbf{1}), \rho \right\} \right] \right. \\ & + \mathcal{C}_{ij} \left[(\mathbf{1} \otimes \sigma_j) \rho (\mathbf{1} \otimes \sigma_i) - \frac{1}{2} \left\{ (\mathbf{1} \otimes \sigma_i \sigma_j), \rho \right\} \right] \\ & + \mathcal{B}_{ij} \left[(\sigma_j \otimes \mathbf{1}) \rho (\mathbf{1} \otimes \sigma_i) - \frac{1}{2} \left\{ (\sigma_j \otimes \sigma_i), \rho \right\} \right] \\ & \left. + \mathcal{B}_{ij}^\dagger \left[(\mathbf{1} \otimes \sigma_j) \rho (\sigma_i \otimes \mathbf{1}) - \frac{1}{2} \left\{ (\sigma_i \otimes \sigma_j), \rho \right\} \right] \right) . \quad (221) \end{aligned}$$

The structure of the various contributions reveals their direct physical meaning. Indeed, the first two contributions are dissipative terms that affect the first, respectively the second, atom in absence of the other. On the contrary, the last two pieces represent the way in which the noise generated by the external fields may correlate the two, otherwise independent, atoms; this effect is present only if the matrix \mathcal{B} is different from zero.

Remark 4.6 As in the single atom case, the environment contributions to \mathcal{H}_{eff} and the entries of the matrix $C_{\alpha\beta}$ in (220) can be expressed in terms of the Hilbert, respectively the Fourier transforms of the thermal Wightmann functions. In particular, the matrices $H_{ij}^{(12)}$ in (218) and \mathcal{B}_{ij} in (221) do not vanish only if the bath state ρ_β correlates bath-operators coupled to different atoms, that is, if the expectations $\text{Tr}[\rho_\beta \Phi_i(t) \Psi_j(0)]$ are nonzero. Only in this case, entanglement has a chance to be created by the action of the bath. Indeed, if $H_{ij}^{(12)} = 0$ and $\mathcal{B}_{ij} = 0$, the two atoms evolve independently and initially separable states may become more mixed, but certainly not entangled. \square

In order to investigate whether the thermal bath made of free fields can actually entangle two independent atoms, one can use the partial transposition criterion, that was introduced in Theorem 2.3. In fact, we are dealing here with a couple of two-level systems, and therefore Theorem 2.4 applies. In more precise terms, the environment is not able to create entanglement if and only if the operation of partial transposition preserves the positivity of the state $\rho(t)$ for all times.

From the operational point of view, one then prepares the two subsystems at $t = 0$ in a separable state:

$$\rho(0) = |\varphi\rangle\langle\varphi| \otimes |\psi\rangle\langle\psi| ; \quad (222)$$

without loss of generality, $\rho(0)$ can be taken to be pure: indeed, if the environment is unable to create entanglement out of pure states, it will certainly not entangle their mixtures. Then, one acts with the operation of partial transposition (over the second factor, for sake of definiteness) on both sides of (216). One thus obtains a master equation for the matrix $\tilde{\rho}(t)$, the partially transposed $\rho(t)$, that can be cast in the following form:⁹³

$$\partial_t \tilde{\rho}(t) = -i \left[\tilde{\mathcal{H}}_{\text{eff}}, \tilde{\rho}(t) \right] + \tilde{\mathbb{D}}[\tilde{\rho}(t)] ; \quad (223)$$

here, $\tilde{\mathcal{H}}_{\text{eff}}$ is a new Hamiltonian to which both the unitary and the dissipative term in (216) contribute:

$$\begin{aligned} \tilde{\mathcal{H}}_{\text{eff}} = & \sum_{i=1}^3 H_i^{(1)} (\sigma_i \otimes \mathbf{1}) + \sum_{ij=1}^3 H_i^{(2)} E_{ij} (\mathbf{1} \otimes \sigma_j) \\ & + \sum_{ij=1}^3 \text{Im}(B \cdot E)_{ij} (\sigma_i \otimes \sigma_j) , \end{aligned} \quad (224)$$

where E is the diagonal 3×3 matrix given by: $E = \text{diag}(-1, 1, -1)$. The additional piece $\tilde{\mathbb{D}}[\cdot]$ is of the form (219), but with a new matrix $C \rightarrow \mathcal{E} \cdot \tilde{C} \cdot \mathcal{E}$, where

$$\tilde{C} = \begin{pmatrix} \mathcal{A} & \mathcal{R}e(\mathcal{B}) + iH^{(12)} \\ \mathcal{R}e(\mathcal{B}^T) - iH^{(12)T} & \mathcal{C}^T \end{pmatrix} , \quad (225)$$

$$\mathcal{E} = \begin{pmatrix} \mathbf{1}_3 & 0 \\ 0 & E \end{pmatrix} , \quad (226)$$

and T denotes full matrix transposition, while $H^{(12)}$ is the coefficient matrix in (218).

Although $\tilde{\rho}(t)$ evolves according to a master equation formally of Kossakowski-Lindblad form, the new coefficient matrix \tilde{C} need not be positive. As a consequence, the time-evolution generated by (223) may result to be neither completely positive, nor positive and need not preserve the positivity of the initial state $\tilde{\rho}(0) \equiv \rho(0)$.

Remark 4.7 Notice that both the Hamiltonian and the dissipative terms of the original master equation (216) contribute to the piece $\tilde{\mathbb{D}}[\cdot]$ in (223), the only one that can possibly produce negative eigenvalues. In particular, this makes more transparent the physical mechanism according to which a direct Hamiltonian coupling $H_{\text{eff}}^{(12)}$ among the two systems can induce entanglement (as studied for instance in Refs.[104-109]): on $\tilde{\rho}(t)$, $H_{\text{eff}}^{(12)}$ “acts” as a generic dissipative contribution, which in general does not preserve positivity. \square

In order to check the presence of negative eigenvalues in $\tilde{\rho}(t)$, instead of examining the full equation (223) it is convenient to study the quantity

$$\mathcal{Q}(t) = \langle \chi | \tilde{\rho}(t) | \chi \rangle, \quad (227)$$

where χ is any 4-dimensional vector.⁹³ Assume that an initial separable state $\tilde{\rho}$ has indeed developed a negative eigenvalue crossing the zero value at time t^* . Then, there exists a vector state $|\chi\rangle$ such that $\mathcal{Q}(t^*) = 0$, $\mathcal{Q}(t) > 0$ for $t < t^*$ and $\mathcal{Q}(t) < 0$ for $t > t^*$. The sign of entanglement creation may thus be given by a negative first derivative of $\mathcal{Q}(t)$ at $t = t^*$. Moreover, by assumption, the state $\rho(t^*)$ is separable. Without loss of generality, one can set $t^* = 0$ and, as already remarked, restrict the attention to factorized pure initial states.

In other words, the two atoms, initially prepared in a state $\rho(0) = \tilde{\rho}(0)$ as in (222), will become entangled by the noisy dynamics induced by their independent interaction with the bath if there exists a suitable vector $|\chi\rangle$, such that:

- 1) $\mathcal{Q}(0) = 0$ and
- 2) $\partial_t \mathcal{Q}(0) < 0$.

Note that the vector $|\chi\rangle$ needs to be chosen entangled, since otherwise $\mathcal{Q}(t)$ is never negative.

Remark 4.8 The criterion just stated is clearly sufficient for entanglement creation. In fact, when $\partial_t \mathcal{Q}(0) > 0$ for all choices of the initial state $\rho(0)$ and probe vector $|\chi\rangle$, entanglement can not be generated by the environment, since $\tilde{\rho}$ remains positive. However, the treatment of the case $\partial_t \mathcal{Q}(0) = 0$ requires special care: in order to check entanglement creation, higher order derivatives of \mathcal{Q} , possibly with a time dependent $|\chi\rangle$, need to be examined. \square

A more manageable test of entanglement creation, valid for any probe vector $|\chi\rangle$, can be obtained by a suitable manipulation of the expression $\partial_t \mathcal{Q}(0)$. In the two-dimensional Hilbert spaces pertaining to the two atoms, consider first the orthonormal basis $\{|\varphi\rangle, |\tilde{\varphi}\rangle\}, \{|\psi\rangle, |\tilde{\psi}\rangle\}$, obtained by augmenting with the two states

$|\tilde{\varphi}\rangle$ and $|\tilde{\psi}\rangle$ the ones that define $\rho(0)$ in (222). They can be both unitarily rotated to the standard basis $\{|-\rangle, |+\rangle\}$ of eigenvectors of σ_3 :

$$\begin{aligned} |\varphi\rangle &= U|-\rangle & |\tilde{\varphi}\rangle &= U|+\rangle, \\ |\psi\rangle &= V|-\rangle & |\tilde{\psi}\rangle &= V|+\rangle. \end{aligned} \quad (228)$$

Similarly, the unitary transformations U and V induce orthogonal transformations \mathcal{U} and \mathcal{V} , respectively, on the Pauli matrices:

$$U^\dagger \sigma_i U = \sum_{j=1}^3 \mathcal{U}_{ij} \sigma_j, \quad V^\dagger \sigma_i V = \sum_{j=1}^3 \mathcal{V}_{ij} \sigma_j. \quad (229)$$

Direct computation then shows that $\partial_t \mathcal{Q}(0)$ can be written as a quadratic form in the components of the probe vector $|\chi\rangle$. As a consequence, vectors $|\chi\rangle$ exist making this form negative, *i.e.* $\partial_t \mathcal{Q}(0) < 0$, if and only if its corresponding discriminant is negative; explicitly:

$$\langle u | \mathcal{A} | u \rangle \langle v | \mathcal{C}^T | v \rangle < \left| \langle u | (\mathcal{R}e(\mathcal{B}) + iH^{(12)}) | v \rangle \right|^2. \quad (230)$$

The three-dimensional vectors $|u\rangle$ and $|v\rangle$ contain the information about the starting factorized state (222): their components can be in fact expressed as:

$$u_i = \sum_{j=1}^3 \mathcal{U}_{ij} \langle + | \sigma_j | - \rangle, \quad v_i = \sum_{j=1}^3 \mathcal{V}_{ij} \langle - | \sigma_j | + \rangle. \quad (231)$$

Therefore, the external quantum fields will be able to entangle the two atoms evolving with the Markovian dynamics generated by (216) and characterized by the Kossakowski matrix (220), if there exists an initial state $|\varphi\rangle\langle\varphi| \otimes |\psi\rangle\langle\psi|$, or equivalently orthogonal transformations \mathcal{U} and \mathcal{V} , for which the inequality (230) is satisfied.

The test in (230) is very general and can be applied to all situations in which two independent subsystems are immersed in a common bath. It can be satisfied only if the coupling between the two subsystems induced by the environment through the mixed correlations $\text{Tr}[\rho_\beta \Phi_i \Psi_j]$, encoded in the coefficients of \mathcal{B} and $H^{(12)}$, are sufficiently strong with respect to the remaining contributions.

As already remarked, in the specific case of two atoms in interaction with the same set of external fields, it is physically reasonable to take $\Psi_i = \Phi_i$, so that the just mentioned mixed, environment generated couplings result maximal and equal to the diagonal ones, *i.e.* $\mathcal{A}_{ij} = \mathcal{B}_{ij} = \mathcal{C}_{ij}$.ⁿ Furthermore, in such a case, recalling (174), all field correlations become proportional to the standard, scalar field temperature Wightmann function $G_\beta(x)$ introduced in (175); as a consequence, the three matrices \mathcal{A} , \mathcal{B} and \mathcal{C} in (220) become all equal to the Kossakowski matrix (196) pertaining to a single atom:

$$\mathcal{A}_{ij} = \mathcal{B}_{ij} = \mathcal{C}_{ij} = A \delta_{ij} - iB \epsilon_{ijk} n_k + C n_i n_j. \quad (232)$$

ⁿThis particular choice for the Kossakowski matrix (220) is of relevance also in phenomenological applications; for instance, it is adopted in the analysis of the phenomenon of resonance fluorescence.^{110,14}

In such a situation, also the Hamiltonian pieces (217) and (218) simplify: $H_{\text{eff}}^{(1)}$ and $H_{\text{eff}}^{(2)}$ can be written exactly as the original system Hamiltonian (214), with the frequency ω replaced by the renormalized one $\tilde{\omega}$ given in (201), while the direct two-atom coupling term takes the form

$$H_{\text{eff}}^{(12)} = -\frac{i}{2} \sum_{i,j=1}^3 \left\{ [\mathcal{K}_\beta(\omega) + \mathcal{K}_\beta(-\omega)] \delta_{ij} + [2\mathcal{K}_\beta(0) - \mathcal{K}_\beta(\omega) - \mathcal{K}_\beta(-\omega)] n_i n_j \right\} \sigma_i \otimes \sigma_j, \quad (233)$$

with $\mathcal{K}_\beta(\zeta)$ as in (192).

Remark 4.9 Recall that this function can be split as in (194) into a vacuum and temperature dependent piece. Since, as observed there, the temperature dependent contribution to $\mathcal{K}_\beta(\zeta)$ is odd in ζ , one deduces that $H_{\text{eff}}^{(12)}$ does not actually involves $T = 1/\beta$: it is the same Lamb term that would have been generated in the case of a two-atom system in the vacuum. Being interested in temperature induced phenomena, we shall not consider this vacuum generated term any further and concentrate the attention on the effects produced by the dissipative contribution $\mathbb{D}[\rho]$ in (219). \square

Let us then consider again the test for entanglement creation given in (230). Because of condition (232), it now involves just the hermitian 3×3 matrix \mathcal{A}_{ij} . Its expression can be further simplified by choosing $u_i = v_i$ in (231); recalling the definitions (228), (229), this in turns implies $|\psi\rangle = |\tilde{\phi}\rangle$ (in other terms, if in the initial state $\rho(0)$ we choose $|\phi\rangle = |-\rangle$, then $|\psi\rangle$ must be taken to be $|+\rangle$). In this case, (230) simply becomes:

$$|\langle u | \mathcal{I}m(\mathcal{A}) | u \rangle|^2 > 0. \quad (234)$$

As long as \mathcal{A}_{ij} is not real, *i.e.* the parameter B in (232) is nonvanishing, this condition is satisfied for every $|u\rangle$ outside the null eigenspace of $\mathcal{I}m(\mathcal{A})$. Take for instance the initial state $\rho(0) = |-\rangle\langle -| \otimes |+\rangle\langle +|$, so that the three-dimensional vector $|u\rangle$ has components $u_i = \{1, -i, 0\}$; from (232) one easily finds: $|\langle u | \mathcal{I}m(\mathcal{A}) | u \rangle|^2 = (Bn_3)^2$, which is in general non vanishing.

We can thus conclude that entanglement between the two atoms is indeed generated through the weak coupling with the external quantum fields. This happens at the beginning of the time-evolution, as soon as $t > 0$. Note however that the test in (234) is unable to determine the fate of this quantum correlations, as time becomes large. In order to discuss asymptotic entanglement, one has to analyze directly the structure of the dynamics generated by the master equation in (216).

4.4. Two Atom Reduced Dynamics: Entanglement Enhancement

As in the case of the single atom evolution, it is convenient to decompose the 4×4 density matrix $\rho(t)$ describing the state of the two atoms along the Pauli matrices:

$$\rho(t) = \frac{1}{4} \left[\mathbf{1} \otimes \mathbf{1} + \sum_{i=1}^3 \rho_{0i}(t) \mathbf{1} \otimes \sigma_i + \sum_{i=1}^3 \rho_{i0}(t) \sigma_i \otimes \mathbf{1} + \sum_{i,j=1}^3 \rho_{ij}(t) \sigma_i \otimes \sigma_j \right], \quad (235)$$

where the components $\rho_{0i}(t)$, $\rho_{i0}(t)$, $\rho_{ij}(t)$ are all real. Substitution of this expansion in the master equation (216) allows deriving the corresponding evolution equations for the above components of $\rho(t)$. As explained in Remark 4.9, we shall ignore the Hamiltonian piece since it can not give rise to temperature dependent entanglement phenomena, and concentrate on the study of the effects induced by the dissipative part in (221), with the elements of the Kossakowski matrix as in (232).

Let us first observe that when the three submatrices \mathcal{A} , \mathcal{B} and \mathcal{C} in (220) are all equal, the the form of the dissipative contribution in (221) simplifies so that the evolution equation can be rewritten as

$$\frac{\partial \rho(t)}{\partial t} = \mathbb{D}[\rho(t)] = \sum_{i,j=1}^3 \mathcal{A}_{ij} \left[\Sigma_j \rho(t) \Sigma_i - \frac{1}{2} \left\{ \Sigma_i \Sigma_j, \rho(t) \right\} \right], \quad (236)$$

in terms of the following symmetrized two-system operators

$$\Sigma_i = \sigma_i \otimes \mathbf{1} + \mathbf{1} \otimes \sigma_i, \quad i = 1, 2, 3. \quad (237)$$

One easily checks that these operators obey the same $su(2)$ Lie algebra of the Pauli matrices; further, together with

$$S_{ij} = \sigma_i \otimes \sigma_j + \sigma_j \otimes \sigma_i, \quad i, j = 1, 2, 3, \quad (238)$$

they form a closed algebra under matrix multiplication. For later reference, we give below its explicit expression: it can be easily obtained using $\sigma_i \sigma_j = \delta_{ij} + i \sum_{k=1}^3 \varepsilon_{ijk} \sigma_k$:

$$\begin{aligned} \Sigma_i \Sigma_j &= 2 \delta_{ij} \mathbf{1} \otimes \mathbf{1} + i \sum_{k=1}^3 \varepsilon_{ijk} \Sigma_k + S_{ij}, \\ S_{ij} \Sigma_k &= \delta_{ik} \Sigma_j + \delta_{jk} \Sigma_i + i \sum_{l=1}^3 \varepsilon_{ikl} S_{lj} + i \sum_{l=1}^3 \varepsilon_{jkl} S_{il}, \\ \Sigma_k S_{ij} &= \delta_{ik} \Sigma_j + \delta_{jk} \Sigma_i - i \sum_{l=1}^3 \varepsilon_{ikl} S_{lj} - i \sum_{l=1}^3 \varepsilon_{jkl} S_{il}, \\ S_{ij} S_{kl} &= 2(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \mathbf{1} \otimes \mathbf{1} + i \sum_{r=1}^3 \left(\delta_{ik} \varepsilon_{jlr} + \delta_{jk} \varepsilon_{ilr} + \delta_{il} \varepsilon_{jkr} + \delta_{jl} \varepsilon_{ikr} \right) \Sigma_r \\ &\quad - \left(2 \delta_{ij} \delta_{kl} - \delta_{ik} \delta_{jl} - \delta_{il} \delta_{jk} \right) S + 2 \left(\delta_{ij} S_{kl} + \delta_{kl} S_{ij} \right) \\ &\quad - \delta_{ik} S_{jl} - \delta_{il} S_{jk} - \delta_{jk} S_{il} - \delta_{jl} S_{ik}, \end{aligned} \quad (239)$$

where $S \equiv \sum_{r=i}^3 S_{ii}$.

Inserting the explicit expression for \mathcal{A}_{ij} given in (232) into (236) and using the decomposition (235), a straightforward but lengthy calculation allows to derive the following evolution equations for the components of $\rho(t)$:

$$\begin{aligned}
\frac{\partial \rho_{0i}(t)}{\partial t} &= -2 \sum_{k=1}^3 \left\{ \left[(2A + C) \delta_{ik} - C n_i n_k \right] \rho_{0k}(t) - B n_k \rho_{ik}(t) \right\} - 2B(2 + \tau) n_i , \\
\frac{\partial \rho_{i0}(t)}{\partial t} &= -2 \sum_{k=1}^3 \left\{ \left[(2A + C) \delta_{ik} - C n_i n_k \right] \rho_{k0}(t) - B n_k \rho_{ki}(t) \right\} - 2B(2 + \tau) n_i , \\
\frac{\partial \rho_{ij}(t)}{\partial t} &= -4 \left[(2A + C) \rho_{ij}(t) + (A + C) \rho_{ji}(t) - \left((A + C) \delta_{ij} - C n_i n_j \right) \tau \right] \\
&\quad - 4B \left[n_i \rho_{0j}(t) + n_j \rho_{i0}(t) \right] - 2B \left[n_i \rho_{j0}(t) + n_j \rho_{0i}(t) \right] \\
&\quad + 2 \sum_{k=1}^3 \left\{ B \delta_{ij} n_k \left[\rho_{k0}(t) + \rho_{0k}(t) \right] + C n_i n_k \left[\rho_{kj}(t) + 2\rho_{jk}(t) \right] \right. \\
&\quad \left. + C n_j n_k \left[\rho_{ik}(t) + 2\rho_{ki}(t) \right] \right\} - 4C \delta_{ij} \sum_{k,l=1}^3 n_k n_l \rho_{kl}(t) . \tag{240}
\end{aligned}$$

In these formulae, the quantity $\tau = \sum_{i=1}^3 \rho_{ii}$ represents the trace of ρ_{ij} ; it is a constant of motion, as easily seen by taking the trace of both sides of the last equation above. Despite this, the value of τ can not be chosen arbitrarily; the requirement of positivity of the initial density matrix $\rho(0)$ readily implies: $-3 \leq \tau \leq 1$.

The system of first order differential equations in (240) naturally splits into two independent sets, involving the symmetric, $\rho_{(0i)} = \rho_{0i} + \rho_{i0}$, $\rho_{(ij)} = \rho_{ij} + \rho_{ji}$, and antisymmetric, $\rho_{[0i]} = \rho_{0i} - \rho_{i0}$, $\rho_{[ij]} = \rho_{ij} - \rho_{ji}$, variables. By examining the structure of the two sets of differential equations, one can conclude that the antisymmetric variables involve exponentially decaying factors, so that they vanish for large times. Then, using the definitions (237) and (238), the study of the equilibrium states $\hat{\rho}$ of the evolution equation (236) can be limited to density matrices of the form

$$\hat{\rho} = \frac{1}{4} \left[\mathbf{1} \otimes \mathbf{1} + \sum_{i=1}^3 \hat{\rho}_i \Sigma_i + \sum_{i,j=1}^3 \hat{\rho}_{ij} S_{ij} \right] , \tag{241}$$

with $\hat{\rho}_{ij} = \hat{\rho}_{ji}$.

The approach to equilibrium of semigroups whose generator is of the generic Kossakowski-Lindblad form has been studied in general and some rigorous mathematical results are available.^{111,3} We shall present such results by adapting them to the case of the evolution generated by the equation (236).

First of all, one notices that in the case of a finite dimensional Hilbert space, there always exists at least one stationary state $\hat{\rho}_0$: this can be understood by recalling that in finite dimensions the ergodic average of the action of a completely positive one-parameter semigroup on any initial state always exists; the result is clearly a stationary state.

Let us now introduce the operators $\mathcal{V}_i = \sum_{j=1}^3 \mathcal{A}_{ij}^{1/2} \Sigma_j$ (recall that \mathcal{A} is non-negative), so that the r.h.s. of (236) can be rewritten in diagonal form:

$$\mathbb{D}[\rho] = \sum_{i,j=1}^3 \left[\mathcal{V}_j \rho \mathcal{V}_i^\dagger - \frac{1}{2} \{ \mathcal{V}_i^\dagger \mathcal{V}_j, \rho \} \right]. \quad (242)$$

When the set \mathcal{M} formed by all operators that commute with the linear span of $\{\mathcal{V}_i, \mathcal{V}_i^\dagger, i = 1, 2, 3\}$ contains only the identity, one can show that the stationary state $\hat{\rho}_0$ is unique, and of maximal rank. On the other hand, when there are several stationary states, they can be generated in a canonical way from a $\hat{\rho}_0$ with maximal rank using the elements of the set \mathcal{M} .

In the case of the evolution equation (236), \mathcal{M} contains the operator $S \equiv \sum_{i=1}^3 S_{ii}$, besides the identity; indeed, with the help of the algebraic relations in (239), one immediately finds: $[S, \Sigma_i] = 0$. Out of these two elements of \mathcal{M} , one can now construct two mutually orthogonal projection operators:^o

$$P = \frac{1}{4} \left[\mathbf{1} \otimes \mathbf{1} - \frac{S}{2} \right], \quad Q = 1 - P. \quad (243)$$

Then, one can show that any given initial state $\rho(0)$ will be mapped by the evolution (236) into the following equilibrium state:

$$\rho(0) \rightarrow \hat{\rho} = \frac{P \hat{\rho}_0 P}{\text{Tr}[P \hat{\rho}_0 P]} \text{Tr}[P \rho(0)] + \frac{Q \hat{\rho}_0 Q}{\text{Tr}[Q \hat{\rho}_0 Q]} \text{Tr}[Q \rho(0)]. \quad (244)$$

That this state is indeed stationary can be easily proven by recalling that P and Q commute with Σ_i , $i = 1, 2, 3$, and thus with the \mathcal{V}_i as well; therefore, $\mathbb{D}[\hat{\rho}] = 0$, for any $\rho(0)$, as a consequence of $\mathbb{D}[\hat{\rho}_0] = 0$.

The problem of finding all invariant states of the dynamics (236) is then reduced to that of identifying a stationary state $\hat{\rho}_0$ with all eigenvalues nonzero. Although in principle this amounts to solving a linear algebraic equation, in practice it can be rather difficult for general master equations of the form (172). Nevertheless, in the case at hand, the problem can be explicitly solved, yielding:

$$\hat{\rho}_0 = \frac{1}{2} \left(\mathbf{1}_2 - R \vec{n} \cdot \vec{\sigma} \right) \otimes \frac{1}{2} \left(\mathbf{1}_2 - R \vec{n} \cdot \vec{\sigma} \right), \quad (245)$$

where $R = B/A$ is the temperature dependent ratio already introduced in (207): note that $0 \leq R \leq 1$, where the two boundary values correspond to the infinite and zero temperature limits, respectively.

Inserting this result in the expression (244) allows deriving the expression of the set of all equilibrium states of the dynamics (236); as expected, they take the symmetric form of (241), with the nonvanishing components given by:

$$\hat{\rho}_i = -\frac{R}{3 + R^2} (\tau + 3) n_i,$$

^oOne easily checks that P is the projection operator $Q_-^{(2)}$ on one of the maximally entangled Bell states introduced in Example 2.3.

$$\hat{\rho}_{ij} = \frac{1}{2(3+R^2)} \left[(\tau - R^2) \delta_{ij} + R^2(\tau + 3) n_i n_j \right]. \quad (246)$$

These stationary density matrices depend on the initial condition $\rho(0)$ only through the value of the parameter τ , that as already mentioned is a constant of motion for the dynamics in (236).

As we have explicitly shown before, an environment made of the quantum free fields is in general able to initially entangle two independent subsystems weakly interacting with it. Nevertheless, by examining the dynamics of a subsystem made of a single atom, we have also seen that such an environment produce dissipation and noise, leading to effects that generically counteract entanglement production. It is therefore remarkable to find the asymptotic state $\hat{\rho}$ in (246) to be still entangled.

To explicitly show this, one can as before act with the operation of partial transposition on $\hat{\rho}$ to see whether negative eigenvalues are present. Alternatively, one can resort to concurrence as discussed in Section 2; indeed, the expressions in (246) are sufficiently simple to allow a direct evaluation. The use of concurrence has another advantage; it not only signals the presence of entanglement, it also provides a measure of it: its value ranges from zero, for separable states, to one, for fully entangled states, like the Bell states.

As explained in Theorem 2.5, in order to determine the concurrence of any 4×4 density matrix ρ representing the state of two atoms, one computes the eigenvalues of the auxiliary matrix $\rho(\sigma_2 \otimes \sigma_2) \rho^* (\sigma_2 \otimes \sigma_2)$, which turn out to be non-negative; their square roots λ_μ , $\mu = 1, 2, 3, 4$, can be ordered decreasingly in value: $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$. The concurrence of ρ is then defined to be: $\mathcal{C}[\rho] = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\}$.

In the case of the asymptotic state $\hat{\rho}$ in (246), the above mentioned procedure gives:

$$\mathcal{C}[\hat{\rho}] = \max \left\{ \frac{(3 - R^2)}{2(3 + R^2)} \left[\frac{5R^2 - 3}{3 - R^2} - \tau \right], 0 \right\}. \quad (247)$$

This expression is indeed nonvanishing, provided we start with an initial state $\rho(0)$ for which

$$\tau < \frac{5R^2 - 3}{3 - R^2}. \quad (248)$$

The concurrence is therefore a linearly decreasing function of τ , starting from its maximum $\mathcal{C} = 1$ for $\tau = -3$ and reaching zero at $\tau = (5R^2 - 3)/(3 - R^2)$; notice that this ratio is an admissible value for τ , since it is always within the interval $[-1, 1]$ for the allowed values of R .

This result is remarkable, since it implies that the dynamics in (240) not only can initially generate entanglement: it can continue to enhance it even in the asymptotic long time regime.

Example 4.4 As initial state, consider the direct product of two pure states:

$$\rho(0) = \rho_{\vec{x}} \otimes \rho_{\vec{y}} , \quad \rho_{\vec{x}} = \frac{1}{2}(\mathbf{1}_2 + \vec{x} \cdot \vec{\sigma}) , \quad \rho_{\vec{y}} = \frac{1}{2}(\mathbf{1}_2 + \vec{y} \cdot \vec{\sigma}) , \quad (249)$$

where \vec{x} and \vec{y} are two unit vectors. In this case, one easily finds that $\tau = \vec{x} \cdot \vec{y}$, so that, recalling (247) the asymptotic entanglement is maximized when \vec{x} and \vec{y} are collinear and pointing in opposite directions. In this case one explicitly finds:

$$\mathcal{C}[\hat{\rho}] = \frac{2R^2}{3 + R^2} , \quad (250)$$

provided $R \neq 0$. Notice that $\mathcal{C}[\hat{\rho}]$ reaches its maximum value of $1/2$ when $R = 1$, *i.e.* at zero temperature, while it vanishes when the temperature becomes infinitely large, *i.e.* $R = 0$. This has to be expected, since in this case the decoherence effects of the bath become dominant. \square

Furthermore, one can easily check that the phenomenon of entanglement production takes place also when the initial state $\rho(0)$ already has a non-vanishing concurrence. Let us consider the following initial state,

$$\rho(0) = \frac{\varepsilon}{4} \mathbf{1} \otimes \mathbf{1} + (1 - \varepsilon)P , \quad (251)$$

which interpolates between the completely mixed separable state (see Example 2.3) and the projection P in (243). Provided $\varepsilon < 2/3$, this state is entangled, with $\mathcal{C}[\rho(0)] = 1 - 3\varepsilon/2$. As this initial state evolves into its corresponding asymptote $\hat{\rho}$, the difference in concurrence turns out to be

$$\mathcal{C}[\hat{\rho}] - \mathcal{C}[\rho(0)] = \frac{3R^2\varepsilon}{3 + R^2} , \quad (252)$$

which is indeed non vanishing. By direct inspection, one sees that the state P above is a fixed point of the dynamics generated by (240) and therefore it coincides with its corresponding asymptotic state $\hat{\rho}$. This is in agreement with the already observed fact that maximal concurrence require $\tau = -3$.

Remark 4.10 The formalism used to analyze the behaviour of stationary atoms in a thermal field bath can be adapted to study the dynamics of a uniformly accelerating point-like detector through a vacuum scalar field. Indeed, the detector can be modeled as a two-level system, in weak interaction with the external, relativistic quantum field, which plays the role of environment.

In the comoving frame, the detector is seen evolving with a master equation of the form (172) as if it were immersed in a thermal bath, with temperature proportional to its proper acceleration. This phenomenon is known in the literature as the Unruh effect. The discussion of the previous sections suggests that for an accelerating subsystem composed of two, non-interacting two-level atoms, quantum correlations should be generated between the two subsystems as a result of the effective open system dynamics. A detailed treatment, similar to the one outlined in

the last Section,¹¹² precisely confirms that in general the asymptotic density matrix describing the equilibrium state of the two atoms turns out to be entangled. \square

In summary, we have seen that the entanglement generating properties of a bath of quantum fields at finite temperature can be ascertained through the study, with different techniques, of two separate time regimes in the evolution of two subsystems immersed in it. Entanglement production in the short time region is regulated by the properties of the generator of their subdynamics, while asymptotic entanglement is measured by the concurrence of the final equilibrium state.

The same techniques can also be used to study entanglement production in more general environments, for which the two subsystems time-evolution is still generated by master equations of type (236), but with a generic matrix \mathcal{A}_{ij} , not necessarily of the form (232).¹¹³ These extended dynamics are useful in phenomenological applications, in particular in quantum optics:^{14,92} the fact that also in these generalized situations the asymptotic entanglement results non-vanishing may give important feedback for the actual realization of elementary quantum computational devices.

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